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Author Index to Volumes 311–320

- Abbott, J., see Castle, K.J. 318 (2000) 565
- Abe, H., H. Takeo and K.M.T. Yamada, Infrared spectroscopy of CO trapped in an argon matrix revisited 311 (1999) 153
- Abramov, Yu.A., A.V. Volkov and P. Coppens, On the evaluation of molecular dipole moments from multipole refinement of X-ray diffraction data 311 (1999) 81
- Abrol, R., N. Sathyamurthy and M.K. Harbola, Reduced potential energy curves for diatomic molecules and their respective cations 312 (1999) 341
- Abu-Eittah, R.H., H. Moustafa and A.M. Al-Omar, The electronic structure of some acyl azides: cyclic–open tautomerism 318 (2000) 276
- Achatz, U., C. Berg, S. Joos, B.S. Fox, M.K. Beyer, G. Niedner-Schatteburg and V.E. Bondybey, Methane activation by platinum cluster ions in the gas phase: effects of cluster charge on the Pt₄ tetramer 320 (2000) 53
- Achiba, Y., see Kikuchi, K. 319 (2000) 472
- Achleitner, A., see Lau, J.T. 317 (2000) 269
- Adamo, C. and V. Barone, Accurate excitation energies from time-dependent density functional theory: assessing the PBE0 model for organic free radicals 314 (1999) 152
- Adamo, C., see Bienati, M. 311 (1999) 69
- Adams, J.W., R.A. Poovey Jr. and M. Messina, A Gaussian wavepacket approach for including correlation in the time-dependent Hartree wavefunction for short times 315 (1999) 266
- Adhikari, S.K., see Biswas, P.K. 317 (2000) 129
- Agafonov, V., see Senyavin, V.M. 313 (1999) 421
- Agafonov, V., see Céolin, R. 314 (1999) 21
- Agafonov, V., see Allouchi, H. 317 (2000) 40
- Agmon, N., Mechanism of hydroxide mobility 319 (2000) 247
- Agmon, N., see Solntsev, K.M. 320 (2000) 262
- Agreiter, J.K., A.M. Knight and M.A. Duncan, ZEKE-PFI spectroscopy of the Al–(H₂O) and Al–(D₂O) complexes 313 (1999) 162
- Ågren, H., see Engström, M. 319 (2000) 191
- Aguilar, A., see Aquilanti, V. 318 (2000) 619
- Aguillon, F., see Babikov, D. 316 (2000) 129
- Aguirre, F., J. Husband, C.J. Thompson and R.B. Metz, Gas-phase photodissociation of AuCH₂⁺: the dissociation threshold of jet-cooled and rotationally thermalized ions 318 (2000) 466
- Ahmad, I.K., see Bell, I.S. 320 (2000) 311
- Ahmed, M., D.S. Peterka and A.G. Suits, H abstraction dynamics by crossed-beam velocity map imaging: Cl + CH₃OH → CH₂OH + HCl 317 (2000) 264
- Ahmed, M., see Peterka, D.S. 312 (1999) 108
- Ahn, B.U., see Lee, S.K. 320 (2000) 601

- Aichele, K., see Hathiramani, D. 319 (2000) 13
- Aida, H., see Kato, N. 312 (1999) 115
- Ajithkumar, T.G., see Mahesh, T.S. 319 (2000) 278
- Akao, K., see Amano, T. 311 (1999) 433
- Akasaka, T., S. Okubo, M. Kondo, Y. Maeda, T. Wakahara, T. Kato, T. Suzuki, K. Yamamoto, K. Kobayashi and S. Nagase, Isolation and characterization of two Pr@C_{82} isomers 319 (2000) 153
- Åkesson, E., see Tarnovsky, A.N. 312 (1999) 121
- Akimoto, S., I. Yamazaki, S. Takaichi and M. Mimuro, Excitation relaxation of carotenoids within the S_2 state probed by the femtosecond fluorescence up-conversion method 313 (1999) 63
- Akiyama, K., K. Sueki, T. Kodama, K. Kikuchi, Y. Takigawa, H. Nakahara, I. Ikemoto and M. Katada, New fullerenes of a group IV element: Hf metallofullerenes 317 (2000) 490
- Akiyama, K., see Ichikawa, T. 313 (1999) 129
- Akiyama, K., see Kikuchi, K. 319 (2000) 472
- Akiyama, Y., see Nakano, T. 318 (2000) 614
- Akutsu, H., see Saito, K. 318 (2000) 75
- Al-Omar, A.M., see Abu-Eittah, R.H. 318 (2000) 276
- Alacid, M., see Zúñiga, J. 313 (1999) 670
- Alavi, A., R.M. Lynden-Bell and R.J.C. Brown, The pathway to reorientation in ammonium fluoride 320 (2000) 487
- Albrecht, M., P. Fulde and H. Stoll, An ab initio estimate of correlation effects on the band gap of covalent semiconductors: diamond and silicon 319 (2000) 355
- Alcamí, M., see Luna, A. 320 (2000) 129
- Alcantara Jr., P., see Correia, R.R.B. 313 (1999) 553
- Aleksandrak, K., see Szubiakowski, J. 313 (1999) 473
- Alemán, C. and D. Zanuy, A quantum mechanical study of the ionic interactions in model compounds of polyelectrolyte-surfactant complexes derived from polypeptides 319 (2000) 318
- Alexander, U.N., K.D. King and W.D. Lawrance, Temperature dependence of germylene reactions with acetylene, trimethylsilane, and phenylgermane 319 (2000) 529
- Alexiewicz, W., Ensemble averages for Smoluchowski-Debye rotational diffusion in the presence of a two-angle-dependent reorienting force 320 (2000) 582
- Alijah, A., see Baer, M. 319 (2000) 489
- Alikhani, M.E., Theoretical study of the insertion reaction of zinc, cadmium, and mercury atoms with methane and silane 313 (1999) 608
- Alkorta, I., I. Rozas and J. Elguero, How strong are the complexes between methane radical cation and noble gas atoms? 311 (1999) 281
- Allan, M., see Sergenton, A.-C. 319 (2000) 179
- Alleman, J.L., see Dillon, A.C. 316 (2000) 13
- Allen, T.W., M. Hoyles, S. Kuyucak and S.H. Chung, Molecular and Brownian dynamics study of ion selectivity and conductivity in the potassium channel 313 (1999) 358
- Allouchi, H., D.O. López, M.-F. Gardette, J.L. Tamarit, V. Agafonov, H. Szwarc and R. Céolin, Thermal and mechanical behaviour of the $\text{C}_{60} \cdot 2\text{S}_8$ monoclinic compound 317 (2000) 40
- Allouchi, H., see Senyavin, V.M. 313 (1999) 421
- Allouchi, H., see Céolin, R. 314 (1999) 21
- Almairac, R., see Maurin, G. 312 (1999) 14
- Alonso, J.A., see Boustani, I. 311 (1999) 21
- Alvarez, J.-L., see Tarnovsky, A.N. 312 (1999) 121

- Alvarez, L., A. Righi, T. Guillard, S. Rols, E. Anglaret, D. Laplaze and J.-L. Sauvajol, Resonant Raman study of the structure and electronic properties of single-wall carbon nanotubes 316 (2000) 186
- Alvarez, L., A. Righi, S. Rols, E. Anglaret and J.L. Sauvajol, Excitation energy dependence of the Raman spectrum of single-walled carbon nanotubes 320 (2000) 441
- Alvarez, W.E., see Kitiyanan, B. 317 (2000) 497
- Alvariño, J.M., A. Rodríguez, A. Laganà and M.L. Hernández, Double-well structure and microscopic branching in the $O(^1D) + HCl$ reaction 313 (1999) 299
- Amagishi, Y., see Mahara, H. 317 (2000) 23
- Amano, T., K. Akao, H. Oka and O. Unno, Pressure broadening of O_2 in the $a^1\Delta_g$ state 311 (1999) 433
- Amatatsu, Y., Ab initio study on the electronic structures of stilbene at the conical intersection 314 (1999) 364
- Amiot, C., J. Vergès, J. d'Incan and C. Effantin, The $(3)^1\Pi - (3)^1\Sigma^+$ system of KRb 315 (1999) 55
- Amiot, C., J. Vergès, J. D'Incan and C. Effantin, Corrigendum to: "The $(3)^1\Pi - (3)^1\Sigma^+$ systems of KRb" [Chem. Phys. Lett. 315 (1999) 55–60] 318 (2000) 289
- Ammal, S.S.C., see Shrivastava, K.N. 313 (1999) 279
- Amo, Y. and Y. Tominaga, Low-frequency Raman study of ethanol–water mixture 320 (2000) 703
- Amos, R.D., see Wilson, P.J. 312 (1999) 475
- Amos, R.D., see Van Caillie, C. 317 (2000) 159
- Anderson, L.W., see Peck, J.R. 318 (2000) 476
- Ando, Y., see Nagasawa, Y. 312 (1999) 161
- Andrae, D., M. Reiher and J. Hinze, A comparative study of finite nucleus models for low-lying states of few-electron high-Z atoms 320 (2000) 457
- Andrés, J., see Sambrano, J.R. 317 (2000) 437
- Andrés, J., see Castillo, R. 318 (2000) 270
- Andrés, J., see Safont, V.S. 318 (2000) 361
- Andrews, R., see Sinnott, S.B. 315 (1999) 25
- Andrianov, I., V. Bonačić-Koutecký, M. Hartmann, J. Manz, J. Pittner and K. Sundermann, Ab initio three-dimensional quantum dynamics of Ag_3 clusters in the NeNePo process 318 (2000) 256
- Andrieux, M., see Vivien, L. 312 (1999) 617
- Andriotis, A.N., see Menon, M. 320 (2000) 425
- Angeli, C., R. Cimraglia and J.-P. Malrieu, On a mixed Möller–Plesset Epstein–Nesbet partition of the Hamiltonian to be used in multireference perturbation configuration interaction 317 (2000) 472
- Angeli, F., J.-M. Delaye, T. Charpentier, J.-C. Petit, D. Ghaleb and P. Faucon, Investigation of Al–O–Si bond angle in glass by ^{27}Al 3Q-MAS NMR and molecular dynamics 320 (2000) 681
- Anglaret, E., see Vivien, L. 312 (1999) 617
- Anglaret, E., see Alvarez, L. 316 (2000) 186
- Anglaret, E., see Alvarez, L. 320 (2000) 441
- Ankudinov, A.L., J.J. Rehr and S.R. Bare, Hybridization peaks in Pt–Cl XANES 316 (2000) 495
- Aoiz, F.J., see Martínez-Haya, B. 311 (1999) 159
- Appel, G., O. Böhme, R. Mikalo and D. Schmeißer, The polaron and bipolaron contributions to the electronic structure of polypyrrole films 313 (1999) 411
- Aquilanti, V., G. Capecchi, S. Cavalli, D. De Fazio, P. Palmieri, C. Puzzarini, A. Aguilar, X. Giménez and J.M. Lucas, The $He + H_2^+$ reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern 318 (2000) 619
- Araki, M., see Kurita, N. 313 (1999) 693
- Aratono, Y., see Shevtsov, V. 319 (2000) 535

- Arbuznikov, A.V. and M. Hendrickx, Quantum-chemical study of the geometric and electronic structure of the CoC_2 molecule 320 (2000) 575
- Archibong, E.F. and A. St-Amant, Ab initio and B3LYP-DFT calculations of GaP^- and GaP_2^- : the electron affinities and vibrational frequencies of GaP and GaP_2 316 (2000) 151
- Archontis, G., see Xie, Q. 312 (1999) 237
- Ardelean, I. and R. Kimmich, Demagnetizing field effects on the Hahn echo 320 (2000) 81
- Arepalli, S., C.D. Scott, P. Nikolaev and R.E. Smalley, Electronically excited C_2 from laser photodissociated C_{60} 320 (2000) 26
- Arepalli, S., see Iliev, M.N. 316 (2000) 217
- Ariga, K., see Furukawa, K. 318 (2000) 22
- Aristov, V., D. Conroy and H. Reisler, Symmetry and lifetime of the hydroxymethyl radical in the 3p Rydberg state 318 (2000) 393
- Ariu, M., G. Bongiovanni, M.A. Loi, A. Mura, A. Piaggi, L. Rossi, W. Graupner, F. Meghdadi and G. Leising, Radiative defects and optical response in oriented *para*-hexaphenyl films 313 (1999) 405
- Arkhipov, V.I., see Schweitzer, B. 313 (1999) 57
- Arnold, W., see Hathiramani, D. 319 (2000) 13
- Arnolds, H., C.E.M. Rehbein, G. Roberts, R.J. Levis and D.A. King, Femtosecond near-infrared laser desorption of multilayer benzene on Pt(111): spatial origin of hyperthermal desorption 314 (1999) 389
- Arranz, F.J., F. Borondo and R.M. Benito, Transition from order to chaos in a floppy molecule: LiNC/LiCN 317 (2000) 451
- Arteca, G.A., R.E. Cachau and K. Veluri, Structural complexity of hydrogen-bonded networks 319 (2000) 719
- Asada, T., see Kitaura, K. 312 (1999) 319
- Asada, T., see Kitaura, K. 313 (1999) 701
- Asakura, T., see Nakazawa, Y. 311 (1999) 362
- Ascenzi, D., see Regan, P.M. 315 (1999) 187
- Ashfold, M.N.R., see Regan, P.M. 315 (1999) 187
- Assel, M., R. Laenen and A. Laubereau, Femtosecond solvation dynamics of solvated electrons in neat water 317 (2000) 13
- Astle, N., see Yu, Y. 312 (1999) 455
- Aswal, V.K., see Goyal, P.S. 317 (2000) 6
- Au, F.C.K., see Zhou, X.T. 318 (2000) 58
- Aubert-Frécon, M., see Kowalczyk, P. 314 (1999) 47
- Audebert, P., see Chérioux, F. 319 (2000) 669
- Augustyniak, M.A. and M. Krupski, The temperature dependence of the pressure switching of Jahn-Teller deformation in the deuterated ammonium copper Tutton salt 311 (1999) 126
- Ayotte, P., J.A. Kelley, S.B. Nielsen and M.A. Johnson, Vibrational spectroscopy of the $\text{F}^- \cdot \text{H}_2\text{O}$ complex via argon predissociation: photoinduced, intracluster proton transfer? 316 (2000) 455
- Babcock, G.T., see Himo, F. 313 (1999) 374
- Babikov, D., E.A. Gislason, M. Sizun, F. Aguillon and V. Sidis, Fragmentation of Na_3^+ clusters by He impact: effect of initial cluster temperature on non-adiabatic phenomena 316 (2000) 129
- Babin, V., P. Fabeni, M. Nikl, G.P. Pazzi, I. Sildos, N. Zazubovich and S. Zazubovich, Polarized luminescence of CsPbBr_3 nanocrystals (quantum dots) in CsBr:Pb single crystal 314 (1999) 31
- Baboul, A.G., see Curtiss, L.A. 314 (1999) 101

- Bacelo, D.E. and Y. Ishikawa, Theoretical study of microscopic solvation of LiCl in water clusters: $\text{LiCl}(\text{H}_2\text{O})_n$ ($n = 1-4$) 319 (2000) 679
- Bacher, A., see Hofmann, U. 311 (1999) 41
- Bacon, J.A. and S.T. Pratt, Photoelectron spectroscopy of Rydberg states of the methyl radical 311 (1999) 346
- Bacou, F., see Vivien, L. 312 (1999) 617
- Baek, D.Y., see Lee, S.K. 311 (1999) 36
- Baer, M., Strong isotope effects in the $\text{F} + \text{HD}$ reactions at the low-energy interval: a quantum-mechanical study 312 (1999) 203
- Baer, M. and A. Alijah, Quantized non-adiabatic coupling terms to ensure diabatic potentials 319 (2000) 489
- Bagno, A. and M. Bonchio, Effective core potential DFT calculations of nuclear shielding as a tool for the prediction and assignment of the tungsten chemical shift in mono- and polynuclear complexes 317 (2000) 123
- Bagryanskaya, E.G., see Makarov, T.N. 317 (2000) 252
- Bai, Z., see Suo, Z. 315 (1999) 321
- Bailey, S.R., see Sloan, J. 316 (2000) 191
- Bak, K.L., P. Jørgensen, J. Olsen, T. Helgaker and J. Gauss, Coupled-cluster singles, doubles and triples (CCSDT) calculations of atomization energies 317 (2000) 116
- Bak, K.L., J. Gauss, T. Helgaker, P. Jørgensen and J. Olsen, The accuracy of molecular dipole moments in standard electronic structure calculations 319 (2000) 563
- Bakalova, S., see Enchev, V. 314 (1999) 234
- Bakowski, B., see Barry, H.R. 319 (2000) 125
- Balasubramanian, K., see Feng, P.Y. 318 (2000) 417
- Balbuena, P.B., see Li, T. 317 (2000) 421
- Baldelli, S., see Schnitzer, C. 313 (1999) 416
- Baldwin, L.C., see Sulkes, M. 318 (2000) 448
- Ball, D.W., DFT and G2 calculations on the $\text{NO}_2\text{-H}_2\text{O}$ molecular complex 312 (1999) 306
- Balogh, D.T., see Dos Santos Jr., D.S. 317 (2000) 1
- Balter, A., see Szubiakowski, J. 313 (1999) 473
- Balucani, U., G. Garberoglio, G. Sutmann and R. Vallauri, Analysis of single-molecule dynamics in liquid HF 315 (1999) 109
- Bán, M.I., see Stachó, L.L. 311 (1999) 328
- Ban, T., S. Ter-Avetisyan, R. Beuc, H. Skenderović and G. Pichler, Photoassociation of cesium atoms into the double minimum Cs_2 $3^1\Sigma_u^+$ state 313 (1999) 110
- Bañares, L., see Martínez-Haya, B. 311 (1999) 159
- Bandow, S., see Yudasaka, M. 312 (1999) 155
- Bandrauk, A.D., see Talebpour, A. 313 (1999) 789
- Bandyopadhyay, R., see Mishra, S.R. 317 (2000) 510
- Bansal, M., see Gu, J. 311 (1999) 209
- Bao, G.-W., see Kim, J.S. 315 (1999) 307
- Bao, S., see Soos, Z.G. 319 (2000) 631
- Bär, H.-J., see Müller, M. 311 (1999) 485
- Bar, I., see Melchior, A. 315 (1999) 421
- Baranovski, V.I. and O.V. Sizova, The properties of some organic molecules as free species and as ligands in ruthenium(II) complexes 315 (1999) 130
- Barbe, A., see Tyuterev, V.I.G. 316 (2000) 271
- Bare, S.R., see Ankinin, A.L. 316 (2000) 495

- Barinovs, Ģ., N. Marković and G. Nyman, 3D wavepacket calculations of ozone photodissociation in the Hartley band: convergence of the autocorrelation function 315 (1999) 282
- Barisien, T., see Pham, T.-A. 318 (2000) 459
- Barnes, M.D., see Ford, J.V. 316 (2000) 181
- Barone, V., see Bienati, M. 311 (1999) 69
- Barone, V., see Adamo, C. 314 (1999) 152
- Barone, V., see Gagliardi, L. 320 (2000) 518
- Barrientos, C., P. Redondo and A. Largo, Theoretical study of AlC_3 : linear or cyclic ground state? 320 (2000) 481
- Barrientos, C., see Redondo, P. 315 (1999) 224
- Barrio, M., see Céolin, R. 314 (1999) 21
- Barry, H.R., B. Bakowski, L. Corner, T. Freearge, O.T.W. Hawkins, G. Hancock, R.M.J. Jacobs, R. Peverall and G.A.D. Ritchie, OH detection by absorption of frequency-doubled diode laser radiation at 308 nm 319 (2000) 125
- Barsky, D., see Fellers, R.S. 312 (1999) 548
- Bartel, C., see Huckauf, A. 319 (2000) 265
- Bartels, L., M. Wolf, T. Klamroth, P. Saalfrank, A. Kühnle, G. Meyer and K.-H. Rieder, Atomic-scale chemistry: Desorption of ammonia from Cu(111) induced by tunneling electrons 313 (1999) 544
- Bartholomew, G.P., see Verdal, N. 320 (2000) 95
- Bartlett, R.J., see Perera, S.A. 314 (1999) 381
- Bartlett, R.J., see Musiał, M. 320 (2000) 542
- Bässler, H., see Schweitzer, B. 313 (1999) 57
- Bässler, H., see Harrison, M.G. 313 (1999) 755
- Bastida, A., see Zúñiga, J. 313 (1999) 670
- Baştuğ, T., see Erkoç, Ş. 314 (1999) 203
- Bataiev, M.M., see Scheblykin, I.G. 316 (2000) 37
- Bauer, E., see Schmidt, Th. 318 (2000) 549
- Baumert, T., see Frohn Meyer, T. 312 (1999) 447
- Baumert, T., see Rubner, O. 316 (2000) 585
- Bauschlicher, Jr., C.W. and A. Ricca, The heat of formation of C_2F_4 315 (1999) 449
- Bazan, G.C., see Verdal, N. 320 (2000) 95
- Bazeia, D., see Ventura, E. 320 (2000) 587
- Beaupré, S., see Belletête, M. 316 (2000) 101
- Becker, K.H., see Geiger, H. 314 (1999) 465
- BelBruno, J.J., The structure of Al_nN_n ($n = 2-4$) clusters: a DFT study 313 (1999) 795
- Belkić, D., P.A. Dando, H.S. Taylor and J. Main, Decimated signal diagonalization for obtaining the complete eigenspectra of large matrices 315 (1999) 135
- Bell, I.S., I.K. Ahmad, P.A. Hamilton and P.B. Davies, Detection of the transient molecule HOPO in the gas phase by infrared laser spectroscopy 320 (2000) 311
- Bellert, D., see Kamariotis, A. 316 (2000) 60
- Belletête, M., M. Ranger, S. Beaupré, M. Leclerc and G. Durocher, Conformational, optical and photophysical properties of a substituted terfluorene isolated and incorporated in a polyester 316 (2000) 101
- Bello, I., see Zhou, X.T. 318 (2000) 58
- Belorizky, E., see Favier, A. 320 (2000) 49
- Belosludov, R.V., M. Sluiter, Z.-Q. Li and Y. Kawazoe, Ab initio and lattice dynamics studies of the vibrational and geometrical properties of the molecular complex of hydroquinone and C_{60} 312 (1999) 299

- Benito, R.M., see Arranz, F.J. 317 (2000) 451
- Bennett, D.W., see Chen, J. 313 (1999) 741
- Berberan-Santos, M.N., A. Fedorov, J.P. Conde, C. Godet, T. Heitz and J.E. Bourée,
Photoluminescence intensity and anisotropy decays in amorphous carbon 319 (2000) 113
- Beregovaya, I.V., see Shchegoleva, L.N. 312 (1999) 325
- Berg, C., see Achatz, U. 320 (2000) 53
- Bergt, M., see Rubner, O. 316 (2000) 585
- Bermudez, V.M., Chemisorption of NH_3 on $\text{GaN}(0001)-(1 \times 1)$ 317 (2000) 290
- Bernard, E.J., B.R. Strazisar and H.F. Davis, Excited state dynamics of H_2CN radicals 313 (1999) 461
- Bernier, P., see Maurin, G. 312 (1999) 14
- Bernier, P., see Vivien, L. 312 (1999) 617
- Bernshtein, V. and I. Oref, Intramolecular energy redistribution in C_{60} following high-en-
ergy collisions with Li^+ 313 (1999) 52
- Berrah, N., see Yench, A.J. 315 (1999) 37
- Berréhar, J., see Lécuiller, R. 314 (1999) 255
- Berry, A.J., see Mejias, J.A. 314 (1999) 558
- Berthault, P., H. Desvaux, G. Le Goff and M. Péto, A simple way to properly invert
intense nuclear magnetization: application to laser-polarized xenon 314 (1999) 52
- Bessis, D., see Vrinceanu, D. 311 (1999) 395
- Beste, A., see García Hernández, M. 320 (2000) 222
- Bettinelli, M., see Laroche, M. 311 (1999) 167
- Beuc, R., see Ban, T. 313 (1999) 110
- Bevan, J.W., see McIntosh, A. 314 (1999) 57
- Beyer, M.K., see Achatz, U. 320 (2000) 53
- Bezerra Jr., A.G., I.E. Borissevitch, R.E. De Araujo, A.S.L. Gomes and C.B. De Araújo,
Investigation of picosecond optical nonlinearity in porphyrin metal complexes deriva-
tives 318 (2000) 511
- Bhanuprakash, K. and J. Laxmikanth Rao, Theoretical studies on the nonlinear optical
properties of zwitterionic organic molecules: effect of π - σ - π through-bond coupling
on the first hyperpolarizability 314 (1999) 282
- Bhasikuttan, A.C., D.K. Palit, A.V. Sapre and J.P. Mittal, Photophysical characteristics of
diphenyl carbazide-laser flash photolysis and fluorescence studies 316 (2000) 67
- Bhattacharjee, J., see Dutta, A. 314 (1999) 347
- Bhattacharyya, K., see Pal, S.K. 312 (1999) 178
- Bhattacharyya, S.P., see Kumar Mondal, C. 311 (1999) 400
- Bian, W., see Manthe, U. 313 (1999) 647
- Biasioli, F., see Fiegele, T. 316 (2000) 387
- Biczysko, M. and Z. Latajka, The influence of water molecules on the proton position in
 $\text{H}_3\text{N}-\text{HX}$ ($\text{X} = \text{F}, \text{Cl}, \text{Br}$) complexes 313 (1999) 366
- Bienati, M., C. Adamo and V. Barone, Performance of a new hybrid Hartree-
Fock/Kohn-Sham model (B98) in predicting vibrational frequencies, polarisabilities
and NMR chemical shifts 311 (1999) 69
- Biennier, L., see Booth, J.P. 317 (2000) 633
- Bierbaum, V.M., see Li, J. 313 (1999) 76
- Bigot, J.-Y., see Pham, T.-A. 318 (2000) 459
- Billing, G.D., see Zenevich, V.A. 312 (1999) 530
- Binning Jr., R.C., see Ishikawa, Y. 313 (1999) 341

- Birch, D.J.S. and C.D. Geddes, Cluster dynamics, growth and syneresis during silica hydrogel polymerisation 320 (2000) 229
- Biswas, P.K. and S.K. Adhikari, Scattering of positronium by H, He, Ne, and Ar 317 (2000) 129
- Bittererová, M., see Klossika, J.-J. 314 (1999) 182
- Bizzocchi, L., C. Degli Esposti and P. Botschwina, Millimeter-wave spectroscopy of HC_3P isotopomers and coupled-cluster calculations: the molecular structure of phosphabutadiyne 319 (2000) 411
- Bliznyuk, A.A., see Titmuss, S.J. 320 (2000) 169
- Bloß, A., see Durand, Y. 317 (2000) 232
- Bludský, O., P. Nachtigall, J. Hrušák and P. Jensen, The calculation of the vibrational states of SO_2 in the $\tilde{\text{C}}^1\text{B}_2$ electronic state up to the $\text{SO}(\Sigma^-) + \text{O}(\text{P})$ dissociation limit 318 (2000) 607
- Blügel, S., see Heinze, S. 315 (1999) 167
- Blyth, R.I.R., see Duschek, R. 318 (2000) 43
- B.Nagy, J., see Willems, I. 317 (2000) 71
- B.Nagy, J., see Colomer, J.-F. 317 (2000) 83
- Bobrenok, O.F., see Bulgakov, A.V. 320 (2000) 19
- Bodenhausen, G., see Mahesh, T.S. 319 (2000) 278
- Bodor, N. and P. Buchwald, Extended covalent solid forms of carbon dioxide with carbon–oxygen single bonds 319 (2000) 645
- Boens, N., see Molski, A. 318 (2000) 325
- Böhme, O., see Appel, G. 313 (1999) 411
- Böhmer, R., T. Jörg, F. Qi and A. Titze, Stimulated ^7Li echo NMR spectroscopy of slow ionic motions in a solid electrolyte 316 (2000) 419
- Boillot, M.L., see Bousseksou, A. 318 (2000) 409
- Bojarski, P., L. Kulak and J. Kubicki, Donor fluorescence decay in the presence of forward and reverse excitation energy transport in two-component disordered systems 318 (2000) 379
- Bolton, K. and J.B.C. Pettersson, Trapping–desorption and surface penetration of argon on ice 312 (1999) 71
- Bonačić-Koutecký, V., see Andrianov, I. 318 (2000) 256
- Bonadeo, H., see Burgos, E. 320 (2000) 14
- Bonchio, M., see Bagno, A. 317 (2000) 123
- Bondybey, V.E., see Achatz, U. 320 (2000) 53
- Boneß, J., G. Marowsky and H.-G. Rubahn, Growth and thermal destruction of sodium films on $\text{Si}(111)7 \times 7$ surfaces as monitored via second-harmonic generation 313 (1999) 19
- Bongiovanni, G., see Ariu, M. 313 (1999) 405
- Booth, J.P., G. Cunge, L. Biennier, D. Romanini and A. Kachanov, Ultraviolet cavity ring-down spectroscopy of free radicals in etching plasmas 317 (2000) 633
- Borbat, P.P. and J.H. Freed, Multiple-quantum ESR and distance measurements 313 (1999) 145
- Borghs, G., see Jin, Y.D. 320 (2000) 387
- Borissevitch, I.E., see Bezerra Jr., A.G. 318 (2000) 511
- Borondo, F., see Arranz, F.J. 317 (2000) 451
- Borsarelli, C.D., S.E. Braslavsky, M.T. Indelli and F. Scandola, Photophysics of supercomplexes. A laser-induced optoacoustic study of the adducts between $\text{Ru}(\text{bpy})(\text{CN})_3^{2-}$ and polyaza macrocycles 317 (2000) 53
- Bosnick, K.A., An exploration of operator methods in the $\text{E} \otimes \text{e}$ Jahn–Teller problem 317 (2000) 526
- Botschwina, P. and R. Oswald, NC_5NC : results of coupled cluster calculations and an unusual anharmonicity effect 319 (2000) 587
- Botschwina, P., see Bizzocchi, L. 319 (2000) 411

- Bouckaert, S., see Bouwen, W. 314 (1999) 227
- Bourée, J.E., see Berberan-Santos, M.N. 319 (2000) 113
- Bousquet, C., see Maurin, G. 312 (1999) 14
- Bousseksou, A., J.J. McGarvey, F. Varret, J.A. Real, J.-P. Tuchagues, A.C. Dennis and M.L. Boillot, Raman spectroscopy of the high- and low-spin states of the spin crossover complex $\text{Fe(phen)}_2(\text{NCS})_2$: an initial approach to estimation of vibrational contributions to the associated entropy change 318 (2000) 409
- Boustani, I., A. Rubio and J.A. Alonso, Ab initio study of B_{32} clusters: competition between spherical, quasiplanar and tubular isomers 311 (1999) 21
- Bouwen, W., F. Vanhoutte, F. Despa, S. Bouckaert, S. Neukermans, L. Theil Kuhn, H. Weidele, P. Lievens and R.E. Silverans, Stability effects of Au_nX_m^+ ($\text{X} = \text{Cu}, \text{Al}, \text{Y}, \text{In}$) clusters 314 (1999) 227
- Bowden, K., see Škrinářová, Z. 316 (2000) 531
- Bowman, J.M., see Skokov, S. 312 (1999) 494
- Bowman, J.M., see Christoffel, K.M. 315 (1999) 275
- Bowman, M.K., see Samoilova, R.I. 316 (2000) 404
- Boyé, S., see Campos, A. 314 (1999) 91
- Bozek, J.D., see Yench, A.J. 315 (1999) 37
- Bradley, D.D.C., see Hofmann, U. 311 (1999) 41
- Bradley, R.K., see Nikolaev, P. 313 (1999) 91
- Bradshaw, A.M., see Neeb, M. 320 (2000) 217
- Braslavsky, S.E., see Borsarelli, C.D. 317 (2000) 53
- Bravo-Pérez, G., I.L. Garzón and O. Novaro, Non-additive effects in small gold clusters 313 (1999) 655
- Bréchnignac, Ph., see Campos, A. 314 (1999) 91
- Brédas, J.L., see Hill, I.G. 317 (2000) 444
- Breidung, J., J. Demaison, L. Margulès and W. Thiel, Equilibrium structure of SiF_4 313 (1999) 713
- Brettel, K., see Gibasiewicz, K. 315 (1999) 95
- Brickmann, J., see Müller, M. 311 (1999) 485
- Bridgeman, A.J., M.A. Halcrow, M. Jones, E. Krausz and N.K. Solanki, The ground state of a tetragonally compressed copper(II) complex 314 (1999) 176
- Brinkmann, G., P.W. Fowler, D.E. Manolopoulos and A.H.R. Palser, A census of nanotube caps 315 (1999) 335
- Brion, C.E., see Deng, J.K. 313 (1999) 134
- Brock, P.J., see Ruhstaller, B. 317 (2000) 238
- Bronikowski, M.J., see Nikolaev, P. 313 (1999) 91
- Brown, G., see Sloan, J. 316 (2000) 191
- Brown, R.G., see Neuwahl, F.V.R. 319 (2000) 157
- Brown, R.J.C., see Alavi, A. 320 (2000) 487
- Brown, W.A., see Kose, R. 311 (1999) 109
- Brozis, M., see Ottinger, C. 315 (1999) 355
- Brucat, P.J., see Kamaritis, A. 316 (2000) 60
- Brumer, P., see McQuarrie, B.R. 319 (2000) 27
- Bruna, P.J. and F. Grein, Theoretical study of the electron–spin magnetic moment (g -tensor) of FeCl^- 318 (2000) 263
- Brunet, M., see Vivien, L. 312 (1999) 617
- Brunetti, B.G., see Ohoyama, H. 313 (1999) 484
- Brunger, M.J., see El-Zein, A. 319 (2000) 701

- Bruno, D., M. Cacciatore, S. Longo and M. Rutigliano, Gas-surface scattering models for particle fluid dynamics: a comparison between analytical approximate models and molecular dynamics calculations 320 (2000) 245
- Bruno, D., see Longo, S. 316 (2000) 311
- Bryans, T.R., R.E. Wilde, M.W. Holtz and E.L. Quitevis, Autoregressive vibrational-dephasing analysis of the ν_2 band of liquid methyl iodide in nanoporous glass 314 (1999) 459
- Bu, Y., X. Song and C. Liu, Theoretical prediction of the structures and properties of cyclic AlS_2 and GaS_2 systems at density functional theory and all-electron correlation levels 319 (2000) 725
- Buchachenko, A.A., T. González-Lezana, M.I. Hernández, M.P. De Lara Castells, G. Delgado-Barrio and P. Villarreal, Blueshifts of the $\text{B} \leftarrow \text{X}$ excitation spectra of $\text{He}^{79}\text{Br}_2$ using a DIM-based potential 318 (2000) 578
- Buchwald, P., see Bodor, N. 319 (2000) 645
- Budnik, B.A. and R.A. Zubarev, MH^{2+} ion production from protonated polypeptides by electron impact: observation and determination of ionization energies and a cross-section 316 (2000) 19
- Bühl, M., see Heine, T. 316 (2000) 373
- Bulgakov, A.V., O.F. Bobrenok and V.I. Kosyakov, Laser ablation synthesis of phosphorus clusters 320 (2000) 19
- Bulthuis, J., see de Lange, M.J.L. 313 (1999) 491
- Buma, W.J., M. Fanti and F. Zerbetto, Scaling of the second hyperpolarisabilities of conjugated carbon systems: polyynes versus polyenes and fullerenes 313 (1999) 426
- Bunker, P.R. and R.E. Moss, Forbidden electric dipole rotation and rotation-vibration transitions in H_2^+ 316 (2000) 266
- Bunker, P.R., see Osmann, G. 318 (2000) 597
- Burda, C., see Link, S. 315 (1999) 12
- Burgos, E., E. Halac and H. Bonadeo, On the crystal structure of C_{36} 320 (2000) 14
- Burkholder, J.B. and J.J. Orlando, UV absorption cross-sections of *cis*-BrONO 317 (2000) 605
- Bush, S.D., D.E. Rourke, L.G. Kaiser and A. Pines, Relaxation-selective magnetic resonance imaging 311 (1999) 379
- Busnengo, H.F., W. Dong and A. Salin, Six-dimensional classical dynamics of H_2 dissociative adsorption on Pd(111) 320 (2000) 328
- Butkovskaya, N.I. and D.W. Setser, Mechanism for the reaction of hydroxyl radicals with dimethyl disulfide 312 (1999) 37
- Butler, L.J., see Parsons, B. 320 (2000) 499
- Buttet, J., see Félix, C. 313 (1999) 105
- Buttet, J., see Rabin, I. 320 (2000) 59
-
- Cabioc'h, T., E. Thune and M. Jaouen, Carbon-onion thin-film synthesis onto silica substrates 320 (2000) 202
- Cacciatore, M., see Bruno, D. 320 (2000) 245
- Cachau, R.E., see Arteca, G.A. 319 (2000) 719
- Cacialli, F., see Kim, J.S. 315 (1999) 307
- Cai, R., see Qian, W. 319 (2000) 89
- Cai, W.-S., B.-Y. Xia, X.-G. Shao, Q.-X. Guo, B. Maigret and Z.-X. Pan, Stability and geometry prediction for the inclusion complexes of mono- or 1,4-disubstituted benzenes and β -cyclodextrin using a genetic algorithm 319 (2000) 708
- Caleyo, F., see Venegas, V. 318 (2000) 655
- Calvet, L.C., see Chen, J. 313 (1999) 741

- Calzado, C.J. and J.-P. Malrieu, Comparison between explicitly correlated and density functional theory calculations in mixed-valence model systems 317 (2000) 404
- Caminati, W., see Velino, B. 316 (2000) 75
- Caminati, W., see López, J.C. 316 (2000) 81
- Campargue, A. and R. Escribano, Room temperature absorption spectroscopy of GeH₂ near 585 nm 315 (1999) 397
- Campos, A., S. Boyé, Ph. Bréchnignac, S. Douin, C. Fellows, N. Shafizadeh and D. Gauyacq, Vacuum-ultraviolet photodissociation of C₂H₂ via Rydberg states: a study of the fluorescent pathways 314 (1999) 91
- Canuto, S., see Urahata, S. 313 (1999) 235
- Cao, C.-B., see Fu, Q. 314 (1999) 223
- Cao, J., An adiabatic picture for electron transfer in mixed-valence systems 312 (1999) 606
- Cao, P.G., J.L. Yao, B. Ren, B.W. Mao, R.A. Gu and Z.Q. Tian, Surface-enhanced Raman scattering from bare Fe electrode surfaces 316 (2000) 1
- Capaccioli, S., see Corezzi, S. 320 (2000) 113
- Capecchi, G., see Aquilanti, V. 318 (2000) 619
- Capes, L., see Létard, J.-F. 313 (1999) 115
- Capitelli, F., see Capitelli, M. 316 (2000) 517
- Capitelli, M., G. Colonna, M. Catella, F. Capitelli and A. Eletskii, On the relaxation of electron energy distribution function in LIBS plasmas 316 (2000) 517
- Capitelli, M., see Longo, S. 316 (2000) 311
- Capuani, S., L. Mancini, B. Maraviglia, M. Sette and M. Paci, Novel double resonance pulse sequence for low sensitivity nuclei selection 316 (2000) 222
- Carr, D.W., see Chen, J. 313 (1999) 741
- Carrington Jr., T., see Huang, S.-W. 312 (1999) 311
- Carter, S.A., see Ruhstaller, B. 317 (2000) 238
- Carter, V.J., J.P. Kujanpää, F.G. Riddell, P.A. Wright, J.F.C. Turner, C.R.A. Catlow and K.S. Knight, Structure and dynamics of methyl groups in the deuterated microporous organic-inorganic hybrid, aluminium methylphosphonate-β 313 (1999) 505
- Casalboni, M., F. Sarcinelli, R. Pizzoferrato, R. D'Amato, A. Furlani and M.V. Russo, Second-harmonic generation and absorption spectra of platinum organometallic complexes incorporated in PMMA films 319 (2000) 107
- Casalini, R., see Corezzi, S. 320 (2000) 113
- Casanueva, J., see Guilleme, J. 314 (1999) 168
- Castiglioni, C., see Mapelli, C. 314 (1999) 189
- Castillejo, M., see De Nalda, R. 316 (2000) 449
- Castillo, J.F., see Sokolovski, D. 313 (1999) 225
- Castillo, R., V. Moliner and J. Andrés, A theoretical study on the molecular mechanism for the normal Reimer-Tiemann reaction 318 (2000) 270
- Castle, K.J., J. Abbott, X. Peng and W. Kong, Photodissociation of *t*-butyl nitrite between 220 and 250 nm: internal energy distribution of NO 318 (2000) 565
- Castleman Jr., A.W., see Kooi, S.E. 315 (1999) 49
- Castleman Jr., A.W., see Leskiw, B.D. 316 (2000) 31
- Castleman Jr., A.W., see Folmer, D.E. 318 (2000) 637
- Catalán, J., J.C. Del Valle and M. Kasha, Conformity of the 7-azaindole dimer cationic potential with photoionization/Coulomb-explosion MS observations and the concerted biprotonic transfer mechanism 318 (2000) 629
- Catella, M., see Capitelli, M. 316 (2000) 517

- Catlow, C.R.A., see Carter, V.J. 313 (1999) 505
- Cavalli, A., see Dos Santos Jr., D.S. 317 (2000) 1
- Cavalli, S., see Aquilanti, V. 318 (2000) 619
- Cencek, W. and J. Rychlewski, Benchmark calculations for He_2^+ and LiH molecules using explicitly correlated Gaussian functions 320 (2000) 549
- Cencek, W., see Cioslowski, J. 319 (2000) 542
- Céolin, R., J. Li.Tamarit, D.O. López, M. Barrio, V. Agafonov, H. Allouchi, F. Moussa and H. Szwarc, A new hexagonal phase of fullerene C_{60} 314 (1999) 21
- Céolin, R., see Senyavin, V.M. 313 (1999) 421
- Céolin, R., see Allouchi, H. 317 (2000) 40
- Cerullo, G., see Lanzani, G. 313 (1999) 525
- Chakraborty, D., see Maheshwari, S. 315 (1999) 181
- Chakraborty, D.K., see Polavarapu, P.L. 319 (2000) 595
- Chambaud, G., see Panten, D. 311 (1999) 390
- Chamorro, E., see Chattaraj, P.K. 314 (1999) 114
- Champagne, B., see Jacquemin, D. 319 (2000) 327
- Chan, K.S., see Zhu, R.S. 320 (2000) 561
- Chan, S.P., see Liu, Z.F. 318 (2000) 15
- Chan, W.-T. and R. Fournier, Binding of ammonia to small copper and silver clusters 315 (1999) 257
- Chan, W.-T. and I.P. Hamilton, Geometries and vibrational frequencies for calcium and strontium radical salts of C_5H_5 , $\text{C}_5\text{H}_4\text{CH}_3$, $\text{C}_4\text{H}_4\text{N}$, and BH_4 316 (2000) 171
- Chandler, D.W., see Teule, J.M. 320 (2000) 177
- Chandra, A.K., T. Uchimaru, M. Sugie and A. Sekiya, Correlation between hardness and activation energies for reactions of OH radical with halomethanes 318 (2000) 69
- Chang, A.H.H. and S.H. Lin, A theoretical study of the reactions of $\text{S}(^1\text{D}) + \text{H}_2$, HD, D_2 320 (2000) 161
- Chang, C.H., see Chang, R. 317 (2000) 142
- Chang, E.C., see Chang, R. 317 (2000) 142
- Chang, R., J.H. Hsu, W.S. Fann, K.K. Liang, C.H. Chang, M. Hayashi, J. Yu, S.H. Lin, E.C. Chang, K.R. Chuang and S.A. Chen, Experimental and theoretical investigations of absorption and emission spectra of the light-emitting polymer MEH-PPV in solution 317 (2000) 142
- Chang, R., J.H. Hsu, W.S. Fann, J. Yu, S.H. Lin, Y.Z. Lee and S.A. Chen, Aggregated states of luminescent conjugated polymers in solutions 317 (2000) 153
- Chang, Y., see Quitevis, E.L. 319 (2000) 138
- Chaplin, M.F., see Du, Z. 318 (2000) 319
- Chapon, D., see Favier, A. 320 (2000) 49
- Charpentier, T., see Angeli, F. 320 (2000) 681
- Chassé, T., see Zerulla, D. 311 (1999) 8
- Chastanet, G., see Létard, J.-F. 313 (1999) 115
- Châtelet, M., see Vach, H. 314 (1999) 552
- Chattaraj, P.K., E. Chamorro and P. Fuentealba, Chemical bonding and reactivity: a local thermodynamic viewpoint 314 (1999) 114
- Chaudhury, P., see Kumar Mondal, C. 311 (1999) 400
- Cheetham, A.K., see Hsu, W.K. 317 (2000) 77
- Chen, C., see Xiang, J. 315 (1999) 371
- Chen, H.M., see Chen, X.L. 318 (2000) 107
- Chen, J., L.C. Calvet, M.A. Reed, D.W. Carr, D.S. Grubisha and D.W. Bennett, Electronic transport through metal-1,4-phenylene diisocyanide-metal junctions 313 (1999) 741

- Chen, R., G. Ma and H. Guo, Full-dimensional quantum calculation of the vibrational energy levels of hydrogen peroxide (HOOH) 320 (2000) 567
- Chen, S., see Ishigami, M. 319 (2000) 457
- Chen, S.A., see Chang, R. 317 (2000) 142
- Chen, S.A., see Chang, R. 317 (2000) 153
- Chen, T., see Vierheilig, A. 312 (1999) 349
- Chen, X., see Melchior, A. 315 (1999) 421
- Chen, X.J., C.C. Jia, C.K. Xu, G. Ouyang, L.L. Peng, S.X. Tian and K.Z. Xu, An electron momentum spectroscopy study of the highest occupied molecular orbital of chlorotrifluoromethane 319 (2000) 76
- Chen, X.J., see Deng, J.K. 313 (1999) 134
- Chen, X.L., H.M. Chen, J. Li, Y.M. Liu, X.C. Dai, G.H. Sha, J.C. Xie, C.H. Zhang and L. Li, Quantum interference effect on collisional energy transfer within singlet ~ triplet mixed states of $\text{Na}_2 \text{ A}^1\Sigma_u^+(v=8) \sim \text{b}^3\Pi_{ou}(v=14)$ 318 (2000) 107
- Chen, Y., see Palmer, P.M. 318 (2000) 440
- Chen, Y., see Qian, W. 319 (2000) 89
- Chen, Z., S.D. Kennedy and J. Zhong, Theoretical formalism and experimental confirmation of intermolecular dipolar effects under time-averaged magnetic field gradients 313 (1999) 217
- Cheng, L.F., L.S. Liao, W.Y. Lai, X.H. Sun, N.B. Wong, C.S. Lee and S.T. Lee, Effect of deposition rate on the morphology, chemistry and electroluminescence of tris-(8-hydroxyquinoline) aluminum films 319 (2000) 418
- Cherayil, B.J., see Myers, D.J. 313 (1999) 592
- Chergui, M., see Jeannin, C. 316 (2000) 51
- Chérioux, F., H. Maillotte, J.M. Dudley and P. Audebert, Enhancement of non-resonant non-linear refractive index with reduction of absorption in push-pull molecules by reduction of their donor group strength 319 (2000) 669
- Chernozatonskii, L.A., N.R. Serebryanaya and B.N. Mavrin, The superhard crystalline three-dimensional polymerized C_{60} phase 316 (2000) 199
- Chernyak, V., S. Tretiak and S. Mukamel, Electronic versus vibrational optical nonlinearities of push-pull polymers 319 (2000) 261
- Cheskis, S., see Derzy, I. 313 (1999) 121
- Chiang, I.W., see Kelly, K.F. 313 (1999) 445
- Chiba, H., see Ohmori, K. 315 (1999) 411
- Chichinin, A.I., Isotope effects in the deactivation of $\text{O}(^1\text{D})$ atoms by XCl and XF ($\text{X} = \text{H}, \text{D}$) 316 (2000) 425
- Chien, S.-H., see Ma, N.L. 311 (1999) 275
- Chim, R.Y.L., see Jarvis, G.K. 320 (2000) 104
- Chin, B.-C., K. Misawa, T. Masuda and T. Kobayashi, Large static dipole moment in substituted polyacetylenes obtained by electroabsorption 318 (2000) 499
- Chin, S.L., see Talebpour, A. 313 (1999) 789
- Choi, W.B., see Lee, C.J. 312 (1999) 461
- Choi, Y.C., see Lee, C.J. 312 (1999) 461
- Chou, A., see Li, Z. 313 (1999) 313
- Chowdhury, M., see Haldar, M. 312 (1999) 432
- Chowdhury, M., see Haldar, M. 319 (2000) 349
- Chowdhury, P.K., Infrared depletion spectroscopy suggests fast vibrational relaxation in the hydrogen-bonded aniline-tetrahydrofuran ($\text{C}_6\text{H}_5\text{-NH}_2 \cdots \text{OC}_4\text{H}_8$) complex 319 (2000) 501

- Christensen, K.Aa. and F. Jensen, The basis set convergence of the density functional energy for H_2 317 (2000) 400
- Christoffel, K.M., Y. Kim, S. Skokov, J.M. Bowman and S.K. Gray, Quantum and quasiclassical reactive scattering of $O(^1D) + HCl$ using an ab initio potential 315 (1999) 275
- Chu, S.-Y., see Su, M.-D. 320 (2000) 475
- Chua, S.-J., see Pan, J.-F. 315 (1999) 233
- Chuang, K.R., see Chang, R. 317 (2000) 142
- Chung, S.H., see Allen, T.W. 313 (1999) 358
- Chung, S.H., see Corry, B. 320 (2000) 35
- Cimiraglia, R., see Angeli, C. 317 (2000) 472
- Ciobică, I.M., F. Frechard, R.A. van Santen, A.W. Kleyn and J. Hafner, A theoretical study of CH_4 chemisorption on the Ru(0001) surface 311 (1999) 185
- Cioslowski, J., G. Liu and D. Moncrieff, The concerted trimerization of ethyne to benzene revisited 316 (2000) 536
- Cioslowski, J., G. Liu, J. Rychlewski, W. Cencek and J. Komasa, Topology of electron correlation in the $b^3\Sigma_u^+$ state of the H_2 molecule 319 (2000) 542
- Civalleri, B., see Ugliengo, P. 318 (2000) 247
- Claridge, J.B., see Sloan, J. 316 (2000) 191
- Clark, R.J.H., see Hsu, W.K. 317 (2000) 77
- Clary, D.C., see Farebrother, A.J. 319 (2000) 303
- Cleij, T.J., see Sarobe, M. 313 (1999) 31
- Clementi, C., see Regan, P.M. 315 (1999) 187
- Cocchi, M., see Giro, G. 318 (2000) 137
- Cohen, A.J. and N.C. Handy, Assessment of exchange correlation functionals 316 (2000) 160
- Colbert, D.T., see Nikolaev, P. 313 (1999) 91
- Coleman, K.S., see Sloan, J. 316 (2000) 191
- Colliex, C., see Suenaga, K. 316 (2000) 365
- Collins, C., W. Zhou and J. Klinowski, Erratum to "A unique structure of $Cu_2(OH)_3 \cdot NO_3$ crystals in the 'silica garden' and their degradation under electron beam irradiation", [Chem. Phys. Lett. 306 (1999) 145] 312 (1999) 346
- Colomer, J.-F., C. Stephan, S. Lefrant, G. Van Tendeloo, I. Willems, Z. Kónya, A. Fonseca, Ch. Laurent and J. B.Nagy, Large-scale synthesis of single-wall carbon nanotubes by catalytic chemical vapor deposition (CCVD) method 317 (2000) 83
- Colomer, J.-F., see Willems, I. 317 (2000) 71
- Colonna, G., see Capitelli, M. 316 (2000) 517
- Colvin, M., see Fellers, R.S. 312 (1999) 548
- Comoretto, D., see Lanzani, G. 313 (1999) 525
- Conde, J.P., see Berberan-Santos, M.N. 319 (2000) 113
- Cong, Y. and Z.-Z. Yang, General atom-bond electronegativity equalization method and its application in prediction of charge distributions in polypeptide 316 (2000) 324
- Conroy, D., see Aristov, V. 318 (2000) 393
- Constantine, S., see Zhou, Y. 314 (1999) 73
- Coppens, P., see Abramov, Yu.A. 311 (1999) 81
- Corcho, F.J., M. Filizola and J.J. Pérez, Evaluation of the iterative simulated annealing technique in conformational search of peptides 319 (2000) 65
- Corezzi, S., S. Capaccioli, R. Casalini, D. Fioretto, M. Paluch and P.A. Rolla, Check of the temperature- and pressure-dependent Cohen–Grest equation 320 (2000) 113
- Corner, L., see Barry, H.R. 319 (2000) 125

- Cornil, J., see Hill, I.G. 317 (2000) 444
- Correia, R.R.B., P. Alcantara Jr. and S.L.S. Cunha, Dye-induced spectral narrowing of stimulated scattering in CS₂ 313 (1999) 553
- Corry, B., S. Kuyucak and S.H. Chung, Invalidity of continuum theories of electrolytes in nanopores 320 (2000) 35
- Cossart, D. and J.M. Robbe, A comment on the possible fluorescence of CO²⁺ 311 (1999) 248
- Costa, S.M.B., see Levin, P.P. 320 (2000) 194
- Costen, M.L., see Steimle, T.C. 319 (2000) 363
- Cottone, G., R. Noto, G. La Manna and S.L. Fornili, Ab initio study on the photoisomers of a nitro-substituted spiropyran 319 (2000) 51
- Couris, S., see Juha, L. 313 (1999) 431
- Couris, S., see De Nalda, R. 316 (2000) 449
- Couris, S., see Konstantaki, M. 318 (2000) 488
- Cours, T., see Tyuterev, V.I.G. 316 (2000) 271
- Coxon, J.A., see Melville, T.C. 318 (2000) 454
- Cremer, D., see Gräfenstein, J. 316 (2000) 569
- Cremer, D., see He, Y. 317 (2000) 537
- Cronin, T.J., see Zhu, L. 317 (2000) 227
- Császár, A.G., J.S. Kain, O.L. Polyansky, N.F. Zobov, and J. Tennyson, Erratum to "Relativistic correction to the potential energy surface and vibration-rotation levels of water". [Chem. Phys. Lett. 293 (1998) 317] 312 (1999) 613
- Csizmadia, I.G., see Knak Jensen, S.J. 319 (2000) 220
- Cumings, J. and A. Zettl, Mass-production of boron nitride double-wall nanotubes and nanococoons 316 (2000) 211
- Cumings, J. and A. Zettl, Erratum to: "Mass-production of boron nitride double-wall nanotubes and nanococoons" [Chem. Phys. Lett. 316 (2000) 211-216] 318 (2000) 497
- Cumings, J., see Ishigami, M. 319 (2000) 457
- Cummins, P.L., see Titmuss, S.J. 320 (2000) 169
- Cunge, G., see Booth, J.P. 317 (2000) 633
- Cunha, S.L.S., see Correia, R.R.B. 313 (1999) 553
- Cuniberti, C., see Lanzani, G. 313 (1999) 525
- Curik, R., see Gianturco, F.A. 311 (1999) 255
- Curtiss, L.A., P.C. Redfern, K. Raghavachari and J.A. Pople, Gaussian-3 theory: a variation based on third-order perturbation theory and an assessment of the contribution of core-related correlation 313 (1999) 600
- Curtiss, L.A., K. Raghavachari, P.C. Redfern, A.G. Baboul and J.A. Pople, Gaussian-3 theory using coupled cluster energies 314 (1999) 101
- Cvijović, D., see Gandy, P.J.F. 314 (1999) 543
- Da Gama, A.A.S., see De Santana, O.L. 314 (1999) 508
- Dahl, K., see Horng, M.L. 315 (1999) 363
- Dai, L., see Li, D.-C. 316 (2000) 349
- Dai, X.C., see Chen, X.L. 318 (2000) 107
- Dai, Z., X. Yue, B. Peng, Q. Yang, X. Liu and P. Ye, Third-order optical nonlinearities of near-infrared dyes 317 (2000) 9
- D'Amato, R., see Casalboni, M. 319 (2000) 107
- Dando, P.A., see Belkić, D. 315 (1999) 135

- Das, G.P. and D.S. Dudis, An approximate ab initio sum-over-states approach to the calculation of non-linear optical properties in organic molecules 312 (1999) 57
- Das, G.P., see Majumder, C. 311 (1999) 62
- Das, K.K., see Dutta, A. 314 (1999) 347
- Davies, P.B., see Liu, Y. 317 (2000) 181
- Davies, P.B., see Bell, I.S. 320 (2000) 311
- Davis, H.F., see Bernard, E.J. 313 (1999) 461
- Davydov, V.A., see Senyavin, V.M. 313 (1999) 421
- De, R., Y. Fujiwara, T. Haino and Y. Tanimoto, Effect of high magnetic fields on intramolecular exciplex fluorescence of pyrene and dimethylaniline systems 315 (1999) 383
- De Almeida, K.J., see Rocha, W.R. 316 (2000) 510
- De Almeida, W.B., see Rocha, W.R. 316 (2000) 510
- De Almeida, W.B., see Dos Santos, H.F. 319 (2000) 569
- Dean, A.M., see Susnow, R.G. 312 (1999) 262
- De Araújo, C.B., see Bezerra Jr., A.G. 318 (2000) 511
- De Araujo, R.E., see Bezerra Jr., A.G. 318 (2000) 511
- Deb, S.K., see Rao, R. 313 (1999) 749
- Deckert, V., see Stöckle, R.M. 318 (2000) 131
- De Fazio, D., see Aquilanti, V. 318 (2000) 619
- Degenhardt, J. and A.J. McQuillan, Mechanism of oxalate ion adsorption on chromium oxide-hydroxide from pH dependence and time evolution of ATR-IR spectra 311 (1999) 179
- Degli Esposti, C., see Bizzocchi, L. 319 (2000) 411
- De Graaf, C., see Reinhardt, P. 319 (2000) 625
- Delaire, J.A., see Texier, I. 311 (1999) 139
- De Lange, A., see Scheper, C.R. 312 (1999) 131
- De Lange, C.A., see Scheper, C.R. 312 (1999) 131
- De Lange, M.J.L., M. Drabbels, P.T. Griffiths, J. Bulthuis, S. Stolte and J.G. Snijders, Steric asymmetry in state-resolved NO-Ar collisions 313 (1999) 491
- De Lara Castells, M.P., see Buchachenko, A.A. 318 (2000) 578
- Delaye, J.-M., see Angeli, F. 320 (2000) 681
- Delgado-Barrio, G., see Gianturco, F.A. 311 (1999) 255
- Delgado-Barrio, G., see Buchachenko, A.A. 318 (2000) 578
- Dellepiane, G., see Lanzani, G. 313 (1999) 525
- Dell'Erba, A., see Velino, B. 316 (2000) 75
- Dell'Erba, A., see López, J.C. 316 (2000) 81
- Delouis, J.-F., see Texier, I. 311 (1999) 139
- Del Pópolo, M.G., see Leiva, E.P.M. 320 (2000) 393
- Del Re, G., see Rassat, A. 313 (1999) 582
- Del Valle, J.C., see Catalán, J. 318 (2000) 629
- Demaison, J., see Breidung, J. 313 (1999) 713
- De Martino, A., see Vach, H. 314 (1999) 552
- De Melo Mattos, S.V., see Dos Santos, H.F. 319 (2000) 569
- Dem'yanenko, A.V., V.N. Lokhman, D.D. Ogurok, E.A. Ryabov and V.S. Letokhov, Direct observation of S^+ and SF^+ ions resulting from the IR + UV laser irradiation of SF_6 molecules 320 (2000) 594
- De Nalda, R., A. Mavromanolakis, S. Couris and M. Castillejo, Induced $HSiCl$ emission in the UV photodissociation of 2-chloroethenylsilane 316 (2000) 449
- Deng, B., see Lu, Q. 314 (1999) 37

- Deng, H., see Deng, J.K. 313 (1999) 134
- Deng, J.K., G.Q. Li, J.D. Huang, H. Deng, X.D. Wang, F. Wang, Y. He, Y.A. Zhang, C.G. Ning, N.F. Gao, Y. Wang, X.J. Chen, Y. Zheng and C.E. Brion, The valence shell binding energy spectra and frontier orbital momentum profiles of methylpropane (isobutane) by binary ($e, 2e$) spectroscopy 313 (1999) 134
- Denning, R.G., see Thorne, J.R.G. 319 (2000) 185
- Dennis, A.C., see Bousseksou, A. 318 (2000) 409
- De Oliveira, L.F.C., see Dos Santos, H.F. 319 (2000) 569
- Deperasińska, I., see Prochorow, J. 316 (2000) 24
- De P.R. Moreira, I., see Reinhardt, P. 319 (2000) 625
- Deratani, A., see Konstantaki, M. 318 (2000) 488
- Derbyshire, F., see Sinnott, S.B. 315 (1999) 25
- Derzy, I., V.A. Lozovsky and S. Cheskis, Absorption cross-sections and absolute concentration of singlet methylene in methane/air flames 313 (1999) 121
- De Santana, O.L. and A.A.S. Da Gama, Green's function calculation of through-bond electronic coupling in donor-bridge-acceptor model systems 314 (1999) 508
- De Schryver, F., see Molski, A. 318 (2000) 325
- De Schryver, F.C., see Pevenage, D. 319 (2000) 512
- De Silvestri, S., see Lanzani, G. 313 (1999) 525
- De Souza, A.R., see Sambrano, J.R. 317 (2000) 437
- Despa, F., see Bouwen, W. 314 (1999) 227
- Dessent, C.E.H., S.R. Haines and K. Müller-Dethlefs, A new detection scheme for synchronous, high resolution ZEKE and MATI spectroscopy demonstrated on the Phenol · Ar complex 315 (1999) 103
- Dessent, C.E.H., W.D. Geppert, S. Ullrich and K. Müller-Dethlefs, Ionization-induced conformational changes: REMPI and ZEKE spectroscopy of salicyl and benzyl alcohol 319 (2000) 375
- Desseyn, H.O., see Miao, M.S. 316 (2000) 297
- Desvaux, H., see Berthault, P. 314 (1999) 52
- Devdariani, A.Z., see Ohmori, K. 315 (1999) 411
- Dhanabalan, A., see Dos Santos Jr., D.S. 317 (2000) 1
- Dhanya, S., R.D. Saini, P.D. Naik and R.K. Vatsa, Formation of BrO in the photo oxidation of CF_2Br_2 318 (2000) 125
- Dickey, E.C., see Sinnott, S.B. 315 (1999) 25
- Dierksen, G.H.F., see Yamamoto, S. 318 (2000) 590
- Dierksen, G.H.F., see Kellö, V. 319 (2000) 231
- Díez, E., see Guilleme, J. 314 (1999) 168
- Dikanov, S.A., see Gilbert, D.C. 315 (1999) 43
- Dikanov, S.A., see Samoilova, R.I. 316 (2000) 404
- DiLabio, G.A., D.A. Pratt and J.S. Wright, Theoretical calculation of gas-phase ionization potentials for mono- and polysubstituted benzenes 311 (1999) 215
- DiLabio, G.A. and D.R. Matusek, Protonation as a means of manufacturing light trications: a case study of $\text{B}_2\text{H}_3^{3+}$ 317 (2000) 599
- Dillon, A.C., P.A. Parilla, J.L. Alleman, J.D. Perkins and M.J. Heben, Controlling single-wall nanotube diameters with variation in laser pulse power 316 (2000) 13
- Di Marco, P., see Giro, G. 318 (2000) 137
- Dimicoli, I., see Piuze, F. 320 (2000) 282
- D'Incan, J., see Amiot, C. 315 (1999) 55
- D'Incan, J., see Amiot, C. 318 (2000) 289

- Ding, S. and C.A. McDowell, ²³Na Solid-state NMR studies of hydrated disodium adenosine triphosphate 320 (2000) 316
- Ding, W., see Zhang, N. 313 (1999) 69
- Dinger, A., C. Lutterloh and J. Küppers, Kinetics of D abstraction with H atoms from the monodeuteride phase on Si(100) surfaces 311 (1999) 202
- Dinger, A., C. Lutterloh and J. Küppers, Stationary and non-stationary etching of Si(100) surfaces with gas phase and adsorbed hydrogen 320 (2000) 405
- Dinnebier, R.E., see van Smaalen, S. 319 (2000) 283
- Di Palma, T.M., see Satta, M. 316 (2000) 94
- Dixon-Warren, St.J., see Yu, Y. 312 (1999) 455
- Dobek, A., see Gibasiewicz, K. 315 (1999) 95
- Dobkowski, J., V. Galievsky, A. Starukhin and J. Waluk, Relaxation in excited states of porphycene in low-temperature argon and nitrogen matrices 318 (2000) 79
- Doerr, L.H., see Jones, R.H. 319 (2000) 423
- Doetschman, D.C., see Gilbert, D.C. 315 (1999) 43
- Dogariu, A., see Moses, D. 316 (2000) 356
- Dogra, S.K., see Santra, S. 311 (1999) 55
- Doll, K. and N.M. Harrison, Chlorine adsorption on the Cu(111) surface 317 (2000) 282
- Domcke, W., see Sobolewski, A.L. 315 (1999) 293
- Domcke, W., see Krawczyk, R.P. 320 (2000) 535
- Domene, C., P.W. Fowler, P.A. Madden, M. Wilson and R.J. Wheatley, Overlap model and ab initio cluster calculations of polarisabilities of ions in solids 314 (1999) 158
- Domínguez-Adame, F., see Malyshev, V.A. 313 (1999) 255
- Dömötör, G., see Stachó, L.L. 311 (1999) 328
- Donaldson, D.J., see Fono, L. 311 (1999) 131
- Dong, W., see Busnengo, H.F. 320 (2000) 328
- Dong, X., Z. Guilan, W. Haiyan, T. Guoqing and C. Wenju, Study on dynamic optical nonlinearities of excited state proton transfer in ethanol solution of 7-hydroxyquinoline 318 (2000) 433
- Donzé, N., P. Péchy, M. Grätzel, M. Schaer and L. Zuppiroli, Quinolate zinc complexes as electron transporting layers in organic light-emitting diodes 315 (1999) 405
- Dopfer, O., see Olkhov, R.V. 314 (1999) 215
- Doraiswamy, S., see Patwari, G.N. 316 (2000) 433
- Dos Santos, D.A., see Hill, I.G. 317 (2000) 444
- Dos Santos, H.F., H.A. Duarte, R.D. Sinisterra, S.V. De Melo Mattos, L.F.C. De Oliveira and W.B. De Almeida, Quantum-mechanical study of the interaction of α -cyclodextrin with methyl mercury chloride 319 (2000) 569
- Dos Santos Jr., D.S., C.R. Mendonça, D.T. Balogh, A. Dhanabalan, A. Cavalli, L. Misoguti, J.A. Giacometti, S.C. Zilio and O.N. Oliveira Jr., Chromophore aggregation hampers photoisomerization in Langmuir-Blodgett films of stearyl ester of Disperse Red-13 (DR13St) 317 (2000) 1
- Douin, S., see Campos, A. 314 (1999) 91
- Dovesi, R., see Lichanot, A. 318 (2000) 240
- Dovesi, R., see Ugliengo, P. 318 (2000) 247
- Dovesi, R., see Reinhardt, P. 319 (2000) 625
- Drabbel, M., see de Lange, M.J.L. 313 (1999) 491
- Drichko, N.V., see Graja, A. 313 (1999) 725
- Drichko, N.V., see Konarev, D.V. 314 (1999) 570

- Du, X. and Y. Liang, Well-ordered structure of *N*-octadecanoyl-L-alanine Langmuir-Blodgett film studied by FTIR spectroscopy 313 (1999) 565
- Du, Y., see Zhang, N. 313 (1999) 69
- Du, Z., L.J. Dunne, G. Manos and M.F. Chaplin, Exact statistical mechanical treatment of benzene adsorption in a zeolite twin-pore one-dimensional lattice model 318 (2000) 319
- Duan, C., see Liu, Y. 317 (2000) 181
- Duarte, H.A., see Dos Santos, H.F. 319 (2000) 569
- Dudis, D.S., see Das, G.P. 312 (1999) 57
- Dudley, J.M., see Chérioux, F. 319 (2000) 669
- Duer, M.J. and A.J. Painter, Correlating quadrupolar nuclear spins: a multiple-quantum NMR approach 313 (1999) 763
- Duncan, M.A., see Reddic, J.E. 312 (1999) 96
- Duncan, M.A., see Agreiter, J.K. 313 (1999) 162
- Dunin-Borkowski, R.E., see Sloan, J. 316 (2000) 191
- Dunne, L.J., see Du, Z. 318 (2000) 319
- Dunsch, L., see Fedurco, M. 319 (2000) 309
- Durand, Y., A. Bloëß, A.M. van Oijen, J. Köhler, E.J.J. Groenen and J. Schmidt, An optical study of single pentacene molecules in *n*-tetradecane 317 (2000) 232
- Durocher, G., see Belletête, M. 316 (2000) 101
- Duschek, R., F. Mittendorfer, R.I.R. Blyth, F.P. Netzer, J. Hafner and M.G. Ramsey, The adsorption of aromatics on sp-metals: benzene on Al(111) 318 (2000) 43
- Düsterhöft, C., see Kullie, O. 314 (1999) 307
- Dutta, A., J. Bhattacharjee and K.K. Das, $A^3\Pi_0^+ - X^1\Sigma_0^+$ and $B^3\Pi_1 - X^1\Sigma_0^+$ transitions of GaI: an MRDCI study 314 (1999) 347
- Dutta-Roy, B., see Gangopadhyay, D. 318 (2000) 161
- Echt, O., see Fiegele, T. 316 (2000) 387
- Eddaoudi, H., see Konstantaki, M. 318 (2000) 488
- Edwards, W.D., see Streiff, J.H. 312 (1999) 369
- Effantin, C., see Amiot, C. 315 (1999) 55
- Effantin, C., see Amiot, C. 318 (2000) 289
- Eggeling, J., E.A.H. Griffiths, I.R. Gould and T.S. Jones, Negative ion resonances and vibrational mode selectivity in inelastic electron scattering studies of hydrogen and diethylsilane adsorbed on Si(100) 313 (1999) 805
- Egorov, S.A., A. Yethiraj and J.L. Skinner, Local density enhancement in dilute supercritical solutions 317 (2000) 560
- Ehlert, J., see Fiedor, L. 319 (2000) 145
- Ehrenberg, B., see Juha, L. 313 (1999) 431
- Eichler, A., J. Hafner, A. Groß and M. Scheffler, Rotational effects in the dissociation of H_2 on metal surfaces studied by ab initio quantum-dynamics calculations 311 (1999) 1
- Eisenenthal, K.B., see Salafsky, J.S. 319 (2000) 435
- Eiswirth, M., see Fecher, F. 313 (1999) 205
- Eklund, P.C., see Grimes, C.A. 319 (2000) 460
- Eklund, P.C., see Williams, K.A. 320 (2000) 352
- El-Nahas, A.M., N. Tajima and K. Hirao, Do $Cu^{2+}NH_3$ and $Cu^{2+}OH_2$ exist?: theory confirms 'yes!' 318 (2000) 333
- El-Sayed, M.A., see Link, S. 315 (1999) 12
- El-Sayed, M.A., see Mohamed, M.B. 317 (2000) 519

- El-Zein, A., M.J. Brunger and W.R. Newell, Resonance phenomena in electron impact excitation of the fundamental vibrational modes of water 319 (2000) 701
- Elber, R. and M. Karplus, Reply to the paper by Stachó et al. "On the Elber-Karplus reaction path-following method and related procedures" [Chem. Phys. Lett. 311 (1999) 328] 311 (1999) 335
- Eletsii, A., see Capitelli, M. 316 (2000) 517
- Elguero, J., see Alkorta, I. 311 (1999) 281
- Eliav, E., see Landau, A. 313 (1999) 399
- Elles, C.G. and N.E. Levinger, Reverse micelles solubilizing DMSO and DMSO/water mixtures 317 (2000) 626
- Elsaesser, T., see Hogiu, S. 312 (1999) 407
- Elsaesser, T., see Fiedor, L. 319 (2000) 145
- Emsley, J.W., G.R. Luckhurst and P. Pedrielli, Magnetic field induced alignment of the director in a smectic A phase: surface effects 320 (2000) 255
- Emsley, L., see Sakellariou, D. 319 (2000) 253
- Emura, S., see Inoue, T. 316 (2000) 381
- Enchev, V., S. Bakalova, G. Ivanova and N. Stoyanov, Excited state intramolecular proton transfer in 2-acetylindan-1,3-dione 314 (1999) 234
- Endo, Y., see Tang, J. 315 (1999) 69
- Endo, Y., see Kawashima, Y. 315 (1999) 201
- Endou, A., see Shrivastava, K.N. 313 (1999) 279
- Engel, V., see Ermoshin, V.A. 311 (1999) 146
- Engel, V., see Rubner, O. 316 (2000) 585
- Engström, M., F. Himo and H. Ågren, Ab initio *g*-tensor calculations of the thioether substituted tyrosyl radical in galactose oxidase 319 (2000) 191
- Epstein, I.R., see Kurin-Csörgei, K. 311 (1999) 105
- Eriksson, L.A., see Himo, F. 313 (1999) 374
- Erkoç, Ş., T. Baştuğ, M. Hirata and S. Tachimori, Energetics and structural stability of lanthanum microclusters 314 (1999) 203
- Ermoshin, V.A., G. Flachenecker, A. Materny and V. Engel, Classical simulations on the pump-probe spectroscopy of I₂ encapsulated in DDR porosil 311 (1999) 146
- Ernst, M., H. Zimmermann and B.H. Meier, A simple model for heteronuclear spin decoupling in solid-state NMR 317 (2000) 583
- Ertl, G., see Lin, W.F. 312 (1999) 1
- Ertl, G., see Rabin, I. 312 (1999) 394
- Ertl, G., see Félix, C. 313 (1999) 105
- Ertl, G., see Rabin, I. 320 (2000) 59
- Ervin, K.M., see Shi, Y. 318 (2000) 149
- Eryomin, V.V., I.M. Umanskii and N.E. Kuz'menko, Wavepacket dynamics in the ground electronic state of a diatomic molecule 316 (2000) 303
- Escribano, R., see Campargue, A. 315 (1999) 397
- Esfarjani, K., see Onoe, J. 315 (1999) 19
- Espinosa-García, J., Theoretical enthalpies of formation of ROX (R = H, CH₃; X = F, Cl, Br) compounds 315 (1999) 239
- Espinosa-García, J., Theoretical C-H bond dissociation enthalpies for CH₃OCl and CH₃OBr 316 (2000) 563
- Estrada, E., Connectivity polynomial and long-range contributions in the molecular connectivity model 312 (1999) 556

- Estrada, E., Characterization of 3D molecular structure 319 (2000) 713
- Eswaramoorthy, M., see Govindaraj, A. 317 (2000) 35
- Evangelisti, S., see Gagliardi, L. 320 (2000) 518
- Evans, M., see Shiell, R.C. 315 (1999) 390
- Eve, J.K. and E.M. McCash, Low-temperature adsorption of CO on Cu(111) studied by reflection absorption infrared spectroscopy 313 (1999) 575
- Fabbi, J.C., J.D. Langenberg and M.D. Morse, The $[17.0]^2\Pi_{1/2} \leftarrow X^2\Pi_{1/2}$ system of AlCa 320 (2000) 303
- Fabeni, P., see Babin, V. 314 (1999) 31
- Fabian, W.M.F., see Škrinárová, Z. 316 (2000) 531
- Faeder, J., see Sanov, A. 313 (1999) 812
- Famulari, A., see Pelmenschikov, A. 314 (1999) 496
- Fang, S., see Grimes, C.A. 319 (2000) 460
- Fang, W.-H., see Liu, D. 318 (2000) 291
- Fann, W.S., see Chang, R. 317 (2000) 142
- Fann, W.S., see Chang, R. 317 (2000) 153
- Fantacci, S., F. Maseras and A. Lledós, Why does {p-Bu¹-calix[4]-(OMe)₂(O)₂ZrCl₂} distort away from C_{2v} symmetry? 315 (1999) 145
- Fanti, M., see Buma, W.J. 313 (1999) 426
- Farantos, S.C., see Prosimiti, R. 311 (1999) 241
- Farebrother, A.J., A.J.H.M. Meijer, D.C. Clary and A.J. Fisher, Formation of molecular hydrogen on a graphite surface via an Eley-Rideal mechanism 319 (2000) 303
- Farmanara, P., V. Stert and W. Radloff, Ultrafast photodissociation dynamics of acetone excited by femtosecond 155 nm laser pulses 320 (2000) 697
- Fattori, V., see Giro, G. 318 (2000) 137
- Faucon, P., see Angeli, F. 320 (2000) 681
- Favero, P.G., see Velino, B. 316 (2000) 75
- Favero, P.G., see López, J.C. 316 (2000) 81
- Favier, A., D. Chapon, P.H. Fries, S. Rast and E. Belorizky, Comment on the intermolecular relaxation dispersion at 400, 600, 800 MHz of the (CH₃)₄N⁺ protons in D₂O solutions with paramagnetic [Gd(D₂O)₈]³⁺ complexes 320 (2000) 49
- Fayer, M.D., see Myers, D.J. 312 (1999) 399
- Fayer, M.D., see Myers, D.J. 313 (1999) 592
- Fayer, M.D., see Rector, K.D. 316 (2000) 122
- Fecher, F., P. Strasser, M. Eiswirth, F.W. Schneider and A.F. Münster, Spatial entrainment of patterns during the polymerization of acrylamide in the presence of the methylene blue-sulfide chemical oscillator 313 (1999) 205
- Fedorov, A., see Berberan-Santos, M.N. 319 (2000) 113
- Fedurco, M., K. Klostermann, U. Kirbach, D. Scheller and L. Dunsch, Reactions of photoexcited C₆₀ with weak organic acids. Novel method for the derivatization of fullerenes 319 (2000) 309
- Fel'dman, E.B. and M.G. Rudavets, Regular and erratic quantum dynamics in spin 1/2 rings with an XY Hamiltonian 311 (1999) 453
- Félix, C., C. Sieber, W. Harbich, J. Buttet, I. Rabin, W. Schulze and G. Ertl, Fluorescence and excitation spectra of Ag₄ in an argon matrix 313 (1999) 105
- Felix, C., see Rabin, I. 320 (2000) 59

- Fellers, R.S., D. Barsky, F. Gygi and M. Colvin, An ab initio study of DNA base pair hydrogen bonding: a comparison of plane-wave versus Gaussian-type function methods 312 (1999) 548
- Fellows, C., see Campos, A. 314 (1999) 91
- Feng, D., see Feng, S. 316 (2000) 146
- Feng, D., see Zhang, D. 317 (2000) 430
- Feng, P.Y. and K. Balasubramanian, Potential energy surfaces of electronic states of AlP_2 , Al_2P and their ions 318 (2000) 417
- Feng, S., D. Feng and J. Li, An ab initio study on the insertion reaction of silylenoid H_2SiLiF with H_2 316 (2000) 146
- Ferradini, C., see Jay-Gerin, J.-P. 317 (2000) 388
- Ferrando, R., F. Montalenti, R. Spadacini and G.E. Tommei, Long-jump probabilities in a BGK model for surface diffusion 315 (1999) 153
- Ferreira, M., see Leite, V.B.P. 316 (2000) 343
- Fichou, D., see Knupfer, M. 318 (2000) 585
- Fiedor, L., H. Scheer, C.N. Hunter, F. Tschirschwitz, B. Voigt, J. Ehlert, E. Nibbering, D. Leupold and T. Elsaesser, Introduction of a 60 fs deactivation channel in the photosynthetic antenna LH1 by Ni-bacteriopheophytin *a* 319 (2000) 145
- Fiegele, T., O. Echt, F. Biasioli, C. Mair and T.D. Märk, Surface-induced reactions of C_n^+ , $50 \leq n \leq 60$ 316 (2000) 387
- Field, R.W., see Jacobson, M.P. 320 (2000) 553
- Filatov, M., S. Shaik, M. Woeller, S. Grimme and S.D. Peyerimhoff, Locked alkenes with a short triplet state lifetime 316 (2000) 135
- Filizola, M., see Corcho, F.J. 319 (2000) 65
- Fink, J., see Knupfer, M. 318 (2000) 585
- Fink, M.J., see Sulkes, M. 318 (2000) 448
- Finley, J.P., Diagrammatic CASPT2 using an internally contracted basis 318 (2000) 190
- Fioretto, D., see Corezzi, S. 320 (2000) 113
- Firth, S., see Hsu, W.K. 317 (2000) 77
- Fischer, R.A., see Schäfer, J. 319 (2000) 477
- Fisher, A.J., see Farebrother, A.J. 319 (2000) 303
- Flachenecker, G., see Ermoshin, V.A. 311 (1999) 146
- Fleniken, J., Y. Kim and H. Meyer, Efficient production of vibrationally excited NO using a pulsed molecular beam discharge source 318 (2000) 529
- Fleniken, J., see Kim, Y. 318 (2000) 522
- Flöthmann, H., see Klossika, J.-J. 314 (1999) 182
- Fodor, L., A. Horváth, K.A. Hötzer, S. Walbert and U.E. Steiner, Enhancement of magnetic field effect in $\text{Ru}(\text{bpy})_3^{2+}/\text{MV}^{2+}$ system by $\text{Ru}(\text{bpy})_3^{2+}\text{-Ag}^+$ exciplex formation 316 (2000) 411
- Foggi, P., see Neuwahl, F.V.R. 319 (2000) 157
- Föhlisch, A., J. Hasselström, O. Karis, P. Väterlein, N. Mårtensson, A. Nilsson, C. Heske, M. Stichler, C. Keller, W. Wurth and D. Menzel, Franck-Condon breakdown in core-level photoelectron spectroscopy of chemisorbed CO 315 (1999) 194
- Fokkens, R.H., see Sarobe, M. 313 (1999) 31
- Folmer, D.E., E.S. Wisniewski and A.W. Castleman Jr., Excited state double proton transfer in the 7-azaindole dimer revisited 318 (2000) 637
- Foltynowicz, R.J., W. Rupp, H.G. Hedderich and E.R. Grant, Photoionization spectrum of the B^2A state of HCO 315 (1999) 210

- Fono, L., D.J. Donaldson, R.J. Proos and B.R. Henry, OH overtone spectra and intensities of pernitric acid 311 (1999) 131
- Fonseca, A., see Willems, I. 317 (2000) 71
- Fonseca, A., see Colomer, J.-F. 317 (2000) 83
- Ford, J.V., B.G. Sumpter, D.W. Noid and M.D. Barnes, Observation of size oscillations in poly(ethylene) glycol/electrolyte composite microparticles 316 (2000) 181
- Fornili, S.L., see Cottone, G. 319 (2000) 51
- Fort, E., see Vach, H. 314 (1999) 552
- Fournier, R., see Chan, W.-T. 315 (1999) 257
- Fowler, P.W., T. Heine and A. Troisi, Valencies of a small fullerene: structures and energetics of $C_{24}H_{2m}$ 312 (1999) 77
- Fowler, P.W., see Domene, C. 314 (1999) 158
- Fowler, P.W., see Brinkmann, G. 315 (1999) 335
- Fowler, P.W., see Heine, T. 316 (2000) 373
- Fox, B.S., see Achatz, U. 320 (2000) 53
- Francisco, J.S., see Good, D.A. 313 (1999) 267
- Francisco, J.S., see Hansen, J.C. 314 (1999) 341
- Francisco, J.S., see Guha, S. 319 (2000) 650
- Francisco, J.S., see Li, Z. 320 (2000) 70
- Frantsuzov, P.A., O.A. Igoshin and E.B. Krissinel, Differential approach to the memory-function reaction kinetics 317 (2000) 481
- Fraser, D.G., see Mejias, J.A. 314 (1999) 558
- Frechard, F., see Ciobîcă, I.M. 311 (1999) 185
- Freed, J.H., see Borbat, P.P. 313 (1999) 145
- Freegarde, T., see Barry, H.R. 319 (2000) 125
- Freeman, R., see Linden, N. 311 (1999) 321
- Frenking, G., see García Hernández, M. 320 (2000) 222
- Frenklach, M., see Krokidis, X. 314 (1999) 534
- Freund, H.-J., see Wolter, K. 320 (2000) 206
- Friedman, N., see Ye, T. 314 (1999) 429
- Friedrichs, S., see Sloan, J. 316 (2000) 191
- Friend, R.H., see Kim, J.S. 315 (1999) 307
- Friend, R.H., see Silva, C. 319 (2000) 494
- Fries, P.H., see Favier, A. 320 (2000) 49
- Fritsch, J., see Wolter, K. 320 (2000) 206
- Frohnmeier, T., M. Hofmann, M. Strehle and T. Baumert, Mapping molecular dynamics (Na_2) in intense laser fields: another dimension to femtochemistry 312 (1999) 447
- Frolov, S.V., see Lee, C.W. 314 (1999) 564
- Froudakis, G.E., see Menon, M. 320 (2000) 425
- Fu, Q., C.-B. Cao and H.-S. Zhu, A solvothermal synthetic route to prepare polycrystalline carbon nitride 314 (1999) 223
- Fu, X., see Ignatyev, I.S. 320 (2000) 469
- Fu, X.-Y., see Liu, D. 318 (2000) 291
- Fu, Z., see Zhou, M. 318 (2000) 644
- Fueno, H. and Y. Taniguchi, Ab initio molecular orbital study of the isomerization reaction surfaces of C_3 and C_3^- 312 (1999) 65
- Fuentealba, P. and Y. Simón-Manso, Basis set superposition error in atomic cluster calculations 314 (1999) 108

- Fuentealba, P., see Chattaraj, P.K. 314 (1999) 114
- Fujii, M., see Tomita, S. 316 (2000) 361
- Fujii, M., see Mitsui, M. 317 (2000) 211
- Fujii, R., see Onaka, K. 315 (1999) 75
- Fujii, T., Analysis of products from a C_2H_2/N_2 microwave discharge: new nitrile species 313 (1999) 733
- Fujitaka, K., see Inoue, T. 316 (2000) 381
- Fujiwara, Y., see De, R. 315 (1999) 383
- Fukui, K., see Noid, D.W. 316 (2000) 285
- Fukumoto, Y., H. Koizumi and K. Makoshi, Location of conical intersections by the Pancharatnam connection and the sign-change theorem of Longuet-Higgins: a model calculation with the H_4 potential surface 313 (1999) 283
- Fulde, P., see Albrecht, M. 319 (2000) 355
- Furlani, A., see Casalboni, M. 319 (2000) 107
- Furukawa, K., S.R. Tian, H. Yamauchi, S. Yamazaki, H. Ijiri, K. Ariga and K. Muraoka, Characterization of H-Y zeolite modified by a radio-frequency CF_4 plasma 318 (2000) 22
- Furukawa, K., see Yokoyama, K. 320 (2000) 645
- Furuya, K., K. Ishikawa, A. Matsuo and T. Ogawa, Mass analysis of high-Rydberg fragments produced by electron impact on ethane by use of a pulsed-field-ionization technique 313 (1999) 559
- Furuya, K., K. Ishikawa and T. Ogawa, Mass analysis of polyatomic high-Rydberg fragments produced by electron impact on methane 319 (2000) 335
- Futamata, M., Coadsorbed state of uracil, water and sulfate species on the gold electrode surface 317 (2000) 304
- Gagliardi, L., S. Evangelisti, V. Barone and B.O. Roos, On the dissociation of N_6 into 3 N_2 molecules 320 (2000) 518
- Gale, G.M., G. Gallot and N. Lascoux, Frequency-dependent vibrational population relaxation time of the OH stretching mode in liquid water 311 (1999) 123
- Galievsky, V., see Dobkowski, J. 318 (2000) 79
- Gallot, G., see Gale, G.M. 311 (1999) 123
- Gamba, Z., see Pastorino, C. 319 (2000) 20
- Gamblin, S.D., see Soldán, P. 313 (1999) 379
- Gan, L.-B., see Wei, T.-X. 319 (2000) 7
- Gan, Z., see Wang, Y. 312 (1999) 277
- Ganapathy, S., see Selvan, R. 316 (2000) 205
- Gandy, P.J.F., D. Cvijović, A.L. Mackay and J. Klinowski, Exact computation of the triply periodic D ('diamond') minimal surface 314 (1999) 543
- Gangopadhyay, D., B.N. Ganguly, T. Mukherjee and B. Dutta-Roy, Anti-Arrhenius behaviour in positronium chemistry: a Kramers' turnover? 318 (2000) 161
- Ganguly, B.N., see Gangopadhyay, D. 318 (2000) 161
- Ganière, J.-D., see Lécuyer, R. 314 (1999) 255
- Gao, H., see Liu, Y. 317 (2000) 181
- Gao, N.F., see Deng, J.K. 313 (1999) 134
- Gao, Z.Q., see Zhang, X.H. 320 (2000) 77
- Garberoglio, G., see Balucani, U. 315 (1999) 109
- García, M.A., J. Llopis and S.E. Paje, A simple model for evaluating the optical absorption spectrum from small Au-colloids in sol-gel films 315 (1999) 313
- García-Vela, A., see Juanes-Marcos, J.C. 317 (2000) 59

- García Hernández, M., A. Beste, G. Frenking and F. Illas, Charge decomposition analysis of the chemisorption bond 320 (2000) 222
- Gardecki, J.A., see Zhou, Y. 314 (1999) 73
- Gardette, M.-F., see Allouchi, H. 317 (2000) 40
- Garzón, I.L., see Bravo-Pérez, G. 313 (1999) 655
- Gauss, J., see Bak, K.L. 317 (2000) 116
- Gauss, J., see Bak, K.L. 319 (2000) 563
- Gauyacq, D., see Campos, A. 314 (1999) 91
- Gawandi, V.B., H. Mohan and J.P. Mittal, Role of solute structure on the stability of the OH-adduct of substituted organic sulfides and its transformation to a radical cation 314 (1999) 451
- Gawandi, V.B., H. Mohan and J.P. Mittal, Erratum to: "Role of solute structure on the stability of the OH-adduct of substituted organic sulfides and its transformation to a radical cation". [Chem. Phys. Lett. 314 (1999) 451–458] 318 (2000) 496
- Gdanitz, R.J., Accurately solving the electronic Schrödinger equation of atoms and molecules using explicitly correlated (r_{12})-MR-Cl. The ground state of beryllium dimer (Be_2) 312 (1999) 578
- Ge, M., see Zhu, X. 319 (2000) 85
- Gebauer, W., see Hopmeier, M. 314 (1999) 9
- Geddes, C.D., see Birch, D.J.S. 320 (2000) 229
- Geetha, B. and A.B. Mandal, 2-Dimensional surface properties of ω -methoxy poly(ethylene glycol) macromonomer and homopolymer at the air–water interface 318 (2000) 35
- Geiger, H., T. Maurer and K.H. Becker, OH-initiated degradation mechanism of 1,4-dioxane in the presence of NO_x 314 (1999) 465
- Geise, H.J., see Jin, Y.D. 320 (2000) 387
- Gensch, T., see Molski, A. 318 (2000) 325
- Geppert, W.D., see Dessent, C.E.H. 319 (2000) 375
- Gerber, G., see Rubner, O. 316 (2000) 585
- Gershgoren, E., see Wang, Z. 313 (1999) 155
- Gershgoren, E., see Ye, T. 314 (1999) 429
- Ghaleb, D., see Angeli, F. 320 (2000) 681
- Ghosh, S., see Philip, R. 313 (1999) 719
- Giacometti, J.A., see Dos Santos Jr., D.S. 317 (2000) 1
- Giannotti, C., see Texier, I. 311 (1999) 139
- Gianturco, F.A., F. Paesani, R. Curik, G. Delgado-Barrio, T. Gozález-Lezana, S. Miret-Artes and P. Villareal, Can the LiH molecule bind He atoms? A computational experiment 311 (1999) 255
- Giardini, A., see Satta, M. 316 (2000) 94
- Gibasiewicz, K., K. Brettel, A. Dobek and W. Leibl, Re-examination of primary radical pair recombination in *Rp. viridis* with Q_A reduced 315 (1999) 95
- Giessen, H., see Wegmann, G. 312 (1999) 376
- Giessen, H., see Harrison, M.G. 313 (1999) 755
- Gilbert, A.T.B. and P.M.W. Gill, Decomposition of exchange-correlation energies 312 (1999) 511
- Gilbert, D.C., S.A. Dikanov, D.C. Doetschman and J.A. Smeija, A study of pyridyl nitrosyl iron(II) tetraphenyl $^{15}\text{N}_4$ -porphyrin. NO geometry and spin coupling to the pyrrole nitrogens 315 (1999) 43
- Gill, P.M.W., see Gilbert, A.T.B. 312 (1999) 511
- Gill, P.M.W., see Lee, A.M. 313 (1999) 271
- Gillen, R.C., see Krawczyk, R.P. 320 (2000) 535
- Giménez, X., see Aquilanti, V. 318 (2000) 619

- Gingerich, K.A., see Shim, I. 317 (2000) 338
- Girard, S., see Laroche, M. 311 (1999) 167
- Giro, G., M. Cocchi, J. Kalinowski, P. Di Marco and V. Fattori, Multicomponent emission from organic light emitting diodes based on polymer dispersion of an aromatic diamine and an oxadiazole derivative 318 (2000) 137
- Gislason, E.A., see Babikov, D. 316 (2000) 129
- Glasbeek, M., see Van der Meer, M.J. 320 (2000) 673
- Godbout, J.T., see Verdal, N. 320 (2000) 95
- Godet, C., see Berberan-Santos, M.N. 319 (2000) 113
- Gödicke, B., A. Langenscheidt, H. Meyer and A. Schweig, Formation of persistent contact ion pairs in solid argon 318 (2000) 102
- Godwal, B.K., see Rao, R. 313 (1999) 749
- Goh, K.L., see Tan, T.L. 315 (1999) 82
- Goh, S.H., see Jin, Z. 318 (2000) 505
- Goldbourt, A., P.K. Madhu and S. Vega, Enhanced conversion of triple to single-quantum coherence in the triple-quantum MAS NMR spectroscopy of spin-5/2 nuclei 320 (2000) 448
- Golemme, A., B. Kippelen and N. Peyghambarian, On the mechanism of orientational photorefractivity in polymer dispersed nematics 319 (2000) 655
- Gomes, A.S.L., see Bezerra Jr., A.G. 318 (2000) 511
- Gonçalves, C.P. and J.R. Mohallem, Ab initio isotope simulated dynamics in the adiabatic approximation 320 (2000) 118
- Gong, Q., see Wang, S. 320 (2000) 411
- González-Lezana, T., see Buchachenko, A.A. 318 (2000) 578
- González Velasco, J., A study at the molecular level of the mechanism of surface diffusion at electrode-electrolyte interfaces 313 (1999) 7
- Good, D.A., Y. Li and J.S. Francisco, Location of the first excited states of fluorinated ethers, E143a (CH_3OCF_3), E134 ($\text{CHF}_2\text{OCHF}_2$), and E125 (CHF_2OCF_3) 313 (1999) 267
- Good, D.A., see Li, Z. 320 (2000) 70
- Goodson III, T., see Varnavski, O. 320 (2000) 688
- Gora, R., see Roszak, S. 313 (1999) 198
- Gorecka, J.N., see Gorecki, J. 319 (2000) 173
- Gorecki, J. and J.N. Gorecka, Molecular dynamics simulations of nonequilibrium rate constant in a model exothermic reaction 319 (2000) 173
- Görner, H., see Gurzadyan, G. 319 (2000) 164
- Gorokhovskiy, A.A., see Turukhin, A.V. 317 (2000) 109
- Gould, I.R., see Eggeling, J. 313 (1999) 805
- Govindaraj, A., M. Nath and M. Eswaramoorthy, Studies of C_{60} and C_{70} incorporated in cubic mesoporous silica (MCM-48) 317 (2000) 35
- Govindaraj, A., see Mishra, S.R. 317 (2000) 510
- Govindaraj, A., see Teredesai, P.V. 319 (2000) 296
- Goyal, P.S. and V.K. Aswal, Role of strain field on the rotational tunnelling spectra of NH_4^+ ions in $(\text{NH}_4)_x\text{K}_{1-x}\text{I}$ 317 (2000) 6
- González-Lezana, T., see Gianturco, F.A. 311 (1999) 255
- Goze, C., see Vivien, L. 312 (1999) 617
- Grabowski, I., see Jankowski, K. 311 (1999) 265
- Grabowski, S.J., Study of correlations for dihydrogen bonds by quantum-chemical calculations 312 (1999) 542

- Gräfenstein, J. and D. Cremer, The combination of density functional theory with multi-configuration methods – CAS-DFT 316 (2000) 569
- Graja, A., R. Lipiec, S. Wapłak, S. Król, I. Turowska-Tyrk and N.V. Drichko, Interplay of acceptor molecule shape, crystal structure and physical properties of a new molecular complex $C_{70} \cdot 2[(Ph_3P)AuCl]$ 313 (1999) 725
- Graja, A., see Konarev, D.V. 314 (1999) 570
- Grant, E.R., see Foltynowicz, R.J. 315 (1999) 210
- Grätzel, M., see Donzé, N. 315 (1999) 405
- Graupner, W., see Ariu, M. 313 (1999) 405
- Gray, S.K., see Christoffel, K.M. 315 (1999) 275
- Grayer, V., see Pham, T.-A. 318 (2000) 459
- Gready, J.E., see Titmuss, S.J. 320 (2000) 169
- Green, M.L.H., see Sloan, J. 316 (2000) 191
- Green, N.J.B. and S.H. Robertson, Diffusion equation coefficients for gas-phase energy transfer 314 (1999) 376
- Green Jr., W.H., see Susnow, R.G. 312 (1999) 262
- Grein, F., see Bruna, P.J. 318 (2000) 263
- Grembecka, J., P. Kędzierski and W.A. Sokalski, Non-empirical analysis of the nature of the inhibitor–active-site interactions in leucine aminopeptidase 313 (1999) 385
- Grey, C.P., see Lim, K.H. 312 (1999) 45
- Griffiths, E.A.H., see Eggeling, J. 313 (1999) 805
- Griffiths, P.T., C.J.S.M. Simpson, S. Stolte and M. Towrie, The photodissociation of physisorbed alkyl nitrites. A-doublet population and alignment of desorbed NO 315 (1999) 158
- Griffiths, P.T., see de Lange, M.J.L. 313 (1999) 491
- Grimes, C.A., C. Mungle, D. Kouzoudis, S. Fang and P.C. Eklund, The 500 MHz to 5.50 GHz complex permittivity spectra of single-wall carbon nanotube-loaded polymer composites 319 (2000) 460
- Grimme, S., see Filatov, M. 316 (2000) 135
- Grimmeiss, H.G., see Steinman, E.A. 319 (2000) 1
- Grobert, N., see Hsu, W.K. 317 (2000) 77
- Groenen, E.J.J., see Durand, Y. 317 (2000) 232
- Groenenboom, G.C., see Teule, J.M. 320 (2000) 177
- Groß, A., see Eichler, A. 311 (1999) 1
- Grossi, G., L. Peroncelli and N. Rahman, Statistics of energy levels in the quantum treatment of an elementary reaction 313 (1999) 639
- Grubisha, D.S., see Chen, J. 313 (1999) 741
- Gryczynski, I., see Kuśba, J. 319 (2000) 661
- Gu, F.L., see M. Bishop, D. 317 (2000) 322
- Gu, J., J. Leszczynski and M. Bansal, A new insight into the structure and stability of Hoogsteen hydrogen-bonded G-tetrad: an ab initio SCF study 311 (1999) 209
- Gu, R.A., see Cao, P.G. 316 (2000) 1
- Gu, X., see Zhu, R. 313 (1999) 98
- Gu, Z., see Wang, S. 320 (2000) 411
- Gu, Z., see Okazaki, T. 320 (2000) 435
- Guarnieri, A., see Huckauf, A. 319 (2000) 265
- Güdel, H.U., see Valiente, R. 320 (2000) 639
- Guderian, A., A.F. Münster, M. Jinguji, M. Kraus and F.W. Schneider, Resonant chaos control by light in a chemiluminescent reaction 312 (1999) 440

- Guha, S. and J.S. Francisco, The isomerization of HOObR to HOBrO 319 (2000) 650
- Guidoni, L., see Pham, T.-A. 318 (2000) 459
- Guilan, Z., see Dong, X. 318 (2000) 433
- Guillard, T., see Alvarez, L. 316 (2000) 186
- Guilleme, J., J. San Fabián, J. Casanueva and E. Díez, Vicinal proton–proton coupling constants: MCSCF ab initio calculations of ethane 314 (1999) 168
- Günther, S., see Luerßen, B. 316 (2000) 331
- Günther, S., see Schmidt, Th. 318 (2000) 549
- Guo, H., see Prosimiti, R. 311 (1999) 241
- Guo, H., see Ma, G. 317 (2000) 315
- Guo, H., see Parsons, B. 320 (2000) 499
- Guo, H., see Chen, R. 320 (2000) 567
- Guo, L., Z. Wu, T. Liu, W. Wang and H. Zhu, Synthesis of novel Sb_2O_3 and Sb_2O_5 nanorods 318 (2000) 49
- Guo, Q.-X., see Cai, W.-S. 319 (2000) 708
- Guo, R., see Xu, S.C. 313 (1999) 617
- Guoqing, T., see Dong, X. 318 (2000) 433
- Gupta, S., see Murad, S. 319 (2000) 60
- Gurzadyan, G. and H. Görner, Picosecond transient absorption spectroscopy of *trans*-4-R-4'-nitrostilbenes with R: OMe, NH_2 and NMe_2 319 (2000) 164
- Gustav, K., see Seibold, M. 314 (1999) 65
- Gutman, I., see Koolen, J.H. 320 (2000) 213
- Gutsev, G.L., B.K. Rao, P. Jena, X.-B. Wang and L.-S. Wang, Origin of the unusual stability of MnO_4^- 312 (1999) 598
- Gygi, F., see Fellers, R.S. 312 (1999) 548
- Ha, T.-K., O. Suleimenov and M.T. Nguyen, A quantum chemical study of three isomers of N_{20} 315 (1999) 327
- Ha, T.-K., see Suter, H.U. 311 (1999) 474
- Ha, T.-K., see Nguyen, M.T. 317 (2000) 135
- Haarer, D., see Hofmann, U. 311 (1999) 41
- Haase, W., see Ostrovsky, S.M. 320 (2000) 295
- Habershon, S., see Lanning, O.J. 317 (2000) 296
- Hache, F., see Vivien, L. 312 (1999) 617
- Hadziioannou, G., see Pham, T.-A. 318 (2000) 459
- Hafner, J., see Eichler, A. 311 (1999) 1
- Hafner, J., see Ciobică, I.M. 311 (1999) 185
- Hafner, J., see Duschek, R. 318 (2000) 43
- Haggquist, G.W., see Osuka, A. 313 (1999) 499
- Haines, S.R., see Dessent, C.E.H. 315 (1999) 103
- Haino, T., see De, R. 315 (1999) 383
- Haiyan, W., see Dong, X. 318 (2000) 433
- Haketa, N., see Yokoyama, K. 320 (2000) 645
- Halac, E., see Burgos, E. 320 (2000) 14
- Halas, N.J., see Kelly, K.F. 313 (1999) 445
- Halberstadt, N., see Seong, J. 314 (1999) 501
- Halcrow, M.A., see Bridgeman, A.J. 314 (1999) 176

- Haldar, M. and M. Chowdhury, Magnetic-field effect on the micellar surface-bound benzophenone tetracarboxylic acid-sodium salt in aqueous cetyltrimethylammonium bromide medium 312 (1999) 432
- Haldar, M. and M. Chowdhury, Large magnetic field effect on the radical pair generated from the photo-induced electron transfer from skatole to 2,4,6-triphenyl pyrilium tetrafluoroborate in aqueous SDS micellar medium 319 (2000) 349
- Halkier, A., T. Helgaker, W. Klopper and J. Olsen, Basis-set convergence of the two-electron Darwin term 319 (2000) 287
- Hall, G.E., see Steimle, T.C. 319 (2000) 363
- Hall, R.J., I.H. Hillier and M.A. Vincent, Which density functional should be used to model hydration? 320 (2000) 139
- Hallmeier, K.H., see Zerulla, D. 311 (1999) 8
- Halpern, J.B., see Ochimizu, T. 313 (1999) 451
- Hamilton, I.P., see Chan, W.-T. 316 (2000) 171
- Hamilton, P.A., see Liu, Y. 317 (2000) 181
- Hamilton, P.A., see Bell, I.S. 320 (2000) 311
- Hamplová, V., see Juha, L. 313 (1999) 431
- Han, K.-L., see Zhu, R. 313 (1999) 98
- Han, K.L., see Zhang, R.Q. 319 (2000) 213
- Han, S.Y., see Kim, S.Y. 318 (2000) 63
- Hancock, G., see Barry, H.R. 319 (2000) 125
- Handy, N.C., see Wilson, P.J. 312 (1999) 475
- Handy, N.C., see Cohen, A.J. 316 (2000) 160
- Hansen, J.C., Y. Li, Z. Li and J.S. Francisco, On the mechanism of the BrO + HBr reaction 314 (1999) 341
- Hansen, J.C., see Li, Z. 320 (2000) 70
- Hara, K., see Ito, N. 318 (2000) 118
- Hara, T., see Onoe, J. 315 (1999) 19
- Harata, A., see Zheng, X.-Y. 316 (2000) 6
- Harata, A., see Ito, K. 318 (2000) 1
- Harbich, W., see Félix, C. 313 (1999) 105
- Harbich, W., see Rabin, I. 320 (2000) 59
- Harbola, M.K., see Abrol, R. 312 (1999) 341
- Hare, J.P., see Hsu, W.K. 317 (2000) 77
- Harima, Y., Y. Kunugi, K. Yamashita and M. Shiotani, Determination of mobilities of charge carriers in electrochemically anion-doped polythiophene film 317 (2000) 310
- Harms, G.S., T. Irgartinger, D. Reiss, A. Renn and U.P. Wild, Fluorescence lifetimes of terrylene in solid matrices 313 (1999) 533
- Harris, K.D.M., see Lanning, O.J. 317 (2000) 296
- Harrison, M.G., G. Urbasch, R.F. Mahrt, H. Giessen, H. Bässler and U. Scherf, Two-photon fluorescence and femtosecond two-photon absorption studies of MeLPPP, a ladder-type poly(phenylene) with low intra-chain disorder 313 (1999) 755
- Harrison, N.M., see Doll, K. 317 (2000) 282
- Hartmann, M., see Andrianov, I. 318 (2000) 256
- Harwell, J.H., see Kitiyanan, B. 317 (2000) 497
- Hasegawa, T., J. Nishijo and J. Umemura, Separation of Raman spectra from fluorescence emission background by principal component analysis 317 (2000) 644
- Hashi, Y., see Onoe, J. 315 (1999) 19

- Hashimoto, J., K. Segawa and H. Sakuragi, Effects of a sulfur substituent on the behavior and generation mode of aroyloxy radicals in the photolysis of diaryl peroxides 314 (1999) 261
- Hashimoto, K., see Ohkoshi, S. 314 (1999) 210
- Hashimoto, M., see Yokoyama, K. 320 (2000) 645
- Hasselström, J., see Föhlisch, A. 315 (1999) 194
- Hathiramani, D., P. Scheier, K. Aichele, W. Arnold, K. Huber and E. Salzbom, Scaling behavior of cross-sections for electron-impact multiple-ionization of negatively-charged fullerene ions 319 (2000) 13
- Hatsui, T., see Pettersson, L.G.M. 311 (1999) 299
- Hättig, C., see Jacquemin, D. 319 (2000) 327
- Hauge, R.H., see Kelly, K.F. 313 (1999) 445
- Hawkins, O.T.W., see Barry, H.R. 319 (2000) 125
- Hayashi, M., see Chang, R. 317 (2000) 142
- Hayashi, S., see Tomita, S. 316 (2000) 361
- Hayden, G.W., see Soos, Z.G. 319 (2000) 631
- Hayes, J.M., T. Reinot and G.J. Small, Hole burning properties of aluminum phthalocyanine tetrasulphonate in water-containing poly(2-hydroxyethyl methacrylate) films 312 (1999) 362
- Hayes, T., see Kamariotis, A. 316 (2000) 60
- He, G.-Z., see Zhu, R. 313 (1999) 98
- He, Y. and B.J. Orr, Ringdown and cavity-enhanced absorption spectroscopy using a continuous-wave tunable diode laser and a rapidly swept optical cavity 319 (2000) 131
- He, Y., Z. He and D. Cremer, Size-extensive quadratic CI methods including quadruple excitations: QCISDTQ and QCISDTQ(6) – On the importance of four-electron correlation effects 317 (2000) 537
- He, Y., see Deng, J.K. 313 (1999) 134
- He, Z., see He, Y. 317 (2000) 537
- Head-Gordon, M., see Hirata, S. 314 (1999) 291
- Head-Gordon, M., see Van Voorhis, T. 317 (2000) 577
- Head-Gordon, M., see Maslen, P.E. 319 (2000) 205
- Heben, M.J., see Dillon, A.C. 316 (2000) 13
- Hedderich, H.G., see Foltynowicz, R.J. 315 (1999) 210
- Heeger, A.J., see Moses, D. 316 (2000) 356
- Heffner, S.A., see Mirau, P.A. 313 (1999) 139
- Heilweil, E.J., see Markelz, A.G. 320 (2000) 42
- Hein, J., see Helbig, M. 312 (1999) 415
- Heine, T., M. Bühl, P.W. Fowler and G. Seifert, Modelling the ^{13}C NMR chemical shifts of C_{84} fullerenes 316 (2000) 373
- Heine, T., see Fowler, P.W. 312 (1999) 77
- Heinze, S., X. Nie, S. Blügel and M. Weinert, Electric-field-induced changes in scanning tunneling microscopy images of metal surfaces 315 (1999) 167
- Heitz, T., see Berberan-Santos, M.N. 319 (2000) 113
- Helbig, M., J. Hein and S. Rentsch, Measurement of the nonlinear refractive index n_2 of electronically excited terthiophene 312 (1999) 415
- Helgaker, T., see Bak, K.L. 317 (2000) 116
- Helgaker, T., see Halkier, A. 319 (2000) 287
- Helgaker, T., see Bak, K.L. 319 (2000) 563
- Helgeson, R., see Wang, H.-L. 315 (1999) 173
- Hendrickx, M., see Arbuznikov, A.V. 320 (2000) 575

- Henn, F., see Maurin, G. 312 (1999) 14
- Henriksen, N.E., Molecular alignment and orientation in short pulse laser fields 312 (1999) 196
- Henry, B.R., see Fono, L. 311 (1999) 131
- Heo, J., see Shin, Y.B. 317 (2000) 639
- Hepburn, J.W., see Shiell, R.C. 315 (1999) 390
- Heremans, P.L., see Jin, Y.D. 320 (2000) 387
- Hering, P., see Kleine, D. 312 (1999) 185
- Herman, M., see Herregodts, F. 316 (2000) 460
- Hernández, E., see Seifert, G. 318 (2000) 355
- Hernández, M.I., see Buchachenko, A.A. 318 (2000) 578
- Hernández, M.L., see Alvarriño, J.M. 313 (1999) 299
- Herregodts, F., D. Hurtmans, J. Vander Auwera and M. Herman, Ar-induced pressure effects in the $\nu_1 + 3\nu_3$ absorption band in $^{12}\text{C}_2\text{H}_2$ 316 (2000) 460
- Hertel, D., see Wegmann, G. 312 (1999) 376
- Hertel, T. and G. Moos, Influence of excited electron lifetimes on the electronic structure of carbon nanotubes 320 (2000) 359
- Heßelmann, A. and G. Jansen, Molecular properties from coupled-cluster Brueckner orbitals 315 (1999) 248
- Heske, C., see Föhlich, A. 315 (1999) 194
- Hida, M., see Inoue, T. 316 (2000) 381
- Higo, J., see Ono, S. 312 (1999) 247
- Hikida, T., see Matsushita, Y. 313 (1999) 85
- Hikita, M., see Tomita, S. 316 (2000) 361
- Hildebrandt, P., see Kneip, C. 311 (1999) 479
- Hildenbrand, D.L. and K.H. Lau, Dissociation energy of the PdO molecule 319 (2000) 95
- Hill, I.G., A. Kahn, J. Cornil, D.A. dos Santos and J.L. Brédas, Occupied and unoccupied electronic levels in organic π -conjugated molecules: comparison between experiment and theory 317 (2000) 444
- Hillier, I.H., see Vincent, M.A. 314 (1999) 138
- Hillier, I.H., see Hall, R.J. 320 (2000) 139
- Himo, F., G.T. Babcock and L.A. Eriksson, Tyrosyl radical in galactose oxidase not strongly perturbed by cysteine cross-link 313 (1999) 374
- Himo, F., see Engström, M. 319 (2000) 191
- Hinze, J., see Andrae, D. 320 (2000) 457
- Hippler, M. and M. Quack, Cw cavity ring-down infrared absorption spectroscopy in pulsed supersonic jets: nitrous oxide and methane 314 (1999) 273
- Hirao, K., see Nakano, H. 317 (2000) 90
- Hirao, K., see El-Nahas, A.M. 318 (2000) 333
- Hirao, K., see Kobayashi, Y. 319 (2000) 695
- Hirata, F., see Sethia, A. 315 (1999) 299
- Hirata, F., see Shapovalov, V. 320 (2000) 186
- Hirata, M., see Erkoç, Ş. 314 (1999) 203
- Hirata, S. and M. Head-Gordon, Time-dependent density functional theory within the Tamm-Dancoff approximation 314 (1999) 291
- Hirota, N., see Ukai, A. 319 (2000) 427
- Ho, M.-S., see Sun, Y.-C. 318 (2000) 7
- Ho, P.K.H., see Kim, J.S. 315 (1999) 307
- Hobza, P., see Ryjáček, F. 313 (1999) 393

- Hodgkinson, P., see Sakellariou, D. 319 (2000) 253
- Hoffmann, M.R. and Y.G. Khait, A self-consistent quasidegenerate coupled-cluster theory 311 (1999) 372
- Hofkens, J., see Molski, A. 318 (2000) 325
- Hofmann, M., see Frohnmeier, T. 312 (1999) 447
- Hofmann, U., A. Schreiber, D. Haarer, S.J. Zilker, A. Bacher, D.D.C. Bradley, M. Redecker, M. Inbasekaran, W.W. Wu and E.P. Woo, Investigations on the grating dynamics in a fast photorefractive guest–host polymer 311 (1999) 41
- Hofstein, J.D. and P.M. Johnson, MATI and PIRI studies of the \tilde{X} and \tilde{A} state of *trans*-1,3-butadiene cation 316 (2000) 229
- Hogiu, S., W. Werncke, M. Pfeiffer and T. Elsaesser, Mode specific vibrational kinetics after intramolecular electron transfer studied by picosecond anti-Stokes Raman spectroscopy 312 (1999) 407
- Hohlneicher, G., see Krawczyk, R.P. 320 (2000) 535
- Hohm, U., Higher-order dipole-polarizabilities and intermolecular interaction potential of P_4 clusters obtained from collision-induced light scattering measurements 311 (1999) 117
- Hohwy, M., see Rasmussen, J.T. 314 (1999) 239
- Holleman, I., see van Smaalen, S. 319 (2000) 283
- Holtz, M.W., see Bryans, T.R. 314 (1999) 459
- Homeier, H.H.H., J. Strasser and H. Yersin, Spin-lattice relaxation in metal-organic platinum(II) complexes 316 (2000) 280
- Hong, G., see Wang, F. 316 (2000) 318
- Hopmeier, M., W. Gebauer, M. Oestreich, M. Sokolowski, E. Umbach and R.F. Mahrt, Relaxation dynamics of excitons in thin quaterthiophene films on different substrates 314 (1999) 9
- Horimoto, N., J. Kohno, F. Mafuné and T. Kondow, Ejection mechanism of molecules and neutral clusters from liquid beam under irradiation of IR laser 318 (2000) 536
- Hornig, M.L., K. Dahl, G. Jones II and M. Maroncelli, Electron transfer in a donor-substituted acridinium dye: evidence for dynamical solvent control 315 (1999) 363
- Horton, H.D., see Rakhimov, R.R. 319 (2000) 639
- Horváth, A., see Fodor, L. 316 (2000) 411
- Hoshi, H., see Manaka, T. 317 (2000) 260
- Hosokoshi, Y., see Mukai, K. 311 (1999) 446
- Hötzer, K.A., see Fodor, L. 316 (2000) 411
- Houston, P.L., see Pisano, P.J. 318 (2000) 385
- Hoyles, M., see Allen, T.W. 313 (1999) 358
- Hrušák, J., see Bludský, O. 318 (2000) 607
- Hsu, C.-C., T.-H. Huang, S. Liu, F.-F. Yeh, B.-Y. Jin, J.A. Sattigeri, C.-W. Shiao and T.-Y. Luh, Conformation of substituted poly-norbornene polymers studied by hyper-Rayleigh scattering at 1064 nm 311 (1999) 355
- Hsu, C.-L., E.F. McCullen and R.G. Tobin, Evidence for an adsorbate-dependent mechanism for surface resistivity: formic acid, oxygen and CO on Cu(100) 316 (2000) 336
- Hsu, C.-W., see Shiell, R.C. 315 (1999) 390
- Hsu, J.H., see Chang, R. 317 (2000) 142
- Hsu, J.H., see Chang, R. 317 (2000) 153
- Hsu, W.K., W.Z. Li, Y.Q. Zhu, N. Grobert, M. Terrones, H. Terrones, N. Yao, J.P. Zhang, S. Firth, R.J.H. Clark, A.K. Cheetham, J.P. Hare, H.W. Kroto and D.R.M. Walton, KCl crystallization within the space between carbon nanotube walls 317 (2000) 77
- Hu, A., P. Otto and J. Ladik, Reply to comment on "Relativistic all-electron Hartree–Fock–Dirac calculation of a quasi one-dimensional chain of selenium atoms" 320 (2000) 6

- Hu, J., see Lu, Q. 314 (1999) 37
- Hu, Z.-M. and H. Nakatsuji, Active sites for methanol synthesis on a Zn/Cu(100) catalyst 313 (1999) 14
- Huan, C.H.A., see Zou, Z. 312 (1999) 149
- Huang, C.-H., see Wei, T.-X. 319 (2000) 7
- Huang, H.H., see Zou, Z. 312 (1999) 149
- Huang, J.D., see Deng, J.K. 313 (1999) 134
- Huang, J.D., see Lee, C.W. 314 (1999) 564
- Huang, S., see Li, D.-C. 316 (2000) 349
- Huang, S.-W. and T. Carrington Jr., A comparison of filter diagonalisation methods with the Lanczos method for calculating vibrational energy levels 312 (1999) 311
- Huang, T.-H., see Hsu, C.-C. 311 (1999) 355
- Huang, T.-H., see Wei, T.-H. 314 (1999) 403
- Huang, T.-H., see Wei, T.-H. 318 (2000) 53
- Huang, W., see Pan, J.-F. 315 (1999) 233
- Huang, W., see Wang, S. 320 (2000) 411
- Huang, Z.-E., see Qian, W. 319 (2000) 89
- Huber, J.R., see Suter, H.U. 311 (1999) 474
- Huber, K., see Hathiramani, D. 319 (2000) 13
- Huckauf, A., A. Guarnieri, C. Bartel and D. Lentz, The rotational spectrum of NCCCNC in excited vibrational states 319 (2000) 265
- Hulliger, J., see Quintel, A. 312 (1999) 567
- Hunter, C.N., see Fiedor, L. 319 (2000) 145
- Huo, W.M. and Y.-K. Kim, Use of relativistic effective core potentials in the calculation of total electron-impact ionization cross-sections 319 (2000) 576
- Hurtmans, D., see Herregodts, F. 316 (2000) 460
- Husband, J., see Aguirre, F. 318 (2000) 466
- Hutchison, J.L., see Sloan, J. 316 (2000) 191
- Hüttermann, J., see Samoilova, R.I. 316 (2000) 404
- Hynes, A.J., see Richter, R.C. 319 (2000) 341
-
- Ichihashi, T., see Yudasaka, M. 312 (1999) 155
- Ichikawa, T., K. Akiyama, G. Satoh and H. Koizumi, Thermal emission of alkaline ions from solid electrolyte: evidence of nonstoichiometric reaction 313 (1999) 129
- Igarashi, K., see Yamaguchi, W. 311 (1999) 341
- Igarashi, K., see Yamaguchi, W. 311 (1999) 415
- Ignatyev, I.S., X. Fu and R. Liu, Transition states for inversion and retention of configuration channels in the reactions of alkyl and silyl fluorides with a water molecule 320 (2000) 469
- Igoshin, O.A., see Frantsuzov, P.A. 317 (2000) 481
- Iijima, S., see Yudasaka, M. 312 (1999) 155
- Iijima, S., see Suenaga, K. 316 (2000) 365
- Iiyama, T., see Ohkubo, T. 312 (1999) 191
- Ijiri, H., see Furukawa, K. 318 (2000) 22
- Ikeda, T., T. Kodaira, F. Izumi, T. Kamiyama and K. Ohshima, Neutron powder diffraction study of potassium clusters in zeolite K-LTA 318 (2000) 93
- Ikemoto, I., see Akiyama, K. 317 (2000) 490
- Ikemoto, I., see Kikuchi, K. 319 (2000) 472
- Ikeo, E., see Kitaura, K. 313 (1999) 701

- Iliev, M.N., A.P. Litvinchuk, S. Arepalli, P. Nikolaev and C.D. Scott, Fine structure of the low-frequency Raman phonon bands of single-wall carbon nanotubes 316 (2000) 217
- Illas, F., see Reinhardt, P. 319 (2000) 625
- Illas, F., see García Hernández, M. 320 (2000) 222
- Imanishi, Y., see Miura, Y. 315 (1999) 1
- Imbihl, R., see Luerßen, B. 316 (2000) 331
- Imbihl, R., see Schmidt, Th. 318 (2000) 549
- Inbasekaran, M., see Hofmann, U. 311 (1999) 41
- Indelli, M.T., see Borsarelli, C.D. 317 (2000) 53
- Ingamells, V.E., M.G. Papadopoulos and A.J. Sadlej, Vibrational corrections to static electric properties of diatomics by Numerov–Cooley integration 316 (2000) 541
- Ingólfsson, O., H. Takeo and S. Nonose, Electronic shell model contemplation of the dissociation dynamics of Al_8^+ : a collision-induced dissociation study 311 (1999) 421
- Inoue, K., see Mukai, K. 311 (1999) 446
- Inoue, M., see Inoue, T. 316 (2000) 381
- Inoue, T., Y. Kubozono, S. Kashino, Y. Takabayashi, K. Fujitaka, M. Hida, M. Inoue, T. Kanbara, S. Emura and T. Uruga, Electronic structure of $\text{Eu}@C_{60}$ studied by XANES and UV–VIS absorption spectra 316 (2000) 381
- Inoue, Y., see Kohno, M. 319 (2000) 451
- Irgartinger, T., see Harms, G.S. 313 (1999) 533
- Ishida, T. and G.C. Schatz, A local interpolation scheme using no derivatives in quantum-chemical calculations 314 (1999) 369
- Ishigaki, T., see Kikuchi, K. 319 (2000) 472
- Ishigami, M., J. Cumings, A. Zettl and S. Chen, A simple method for the continuous production of carbon nanotubes 319 (2000) 457
- Ishii, K., see Nakayama, H. 320 (2000) 323
- Ishikawa, K., see Furuya, K. 313 (1999) 559
- Ishikawa, K., see Manaka, T. 317 (2000) 260
- Ishikawa, K., see Furuya, K. 319 (2000) 335
- Ishikawa, M., see Ye, J.Y. 320 (2000) 607
- Ishikawa, Y., R.C. Binning Jr. and N.S. Shramek, Direct ab initio molecular dynamics study of $\text{NO}_2^+ + (\text{H}_2\text{O})_4 \rightarrow \text{HNO}_3(\text{H}_7\text{O}_3^+)$ 313 (1999) 341
- Ishikawa, Y., see Nakazaki, J. 319 (2000) 385
- Ishikawa, Y., see Bacelo, D.E. 319 (2000) 679
- Ishitobi, H., Z. Sekkat and S. Kawata, Quantifying theory of optical orientation processes in spectrally distinguishable photoisomers: application to a spiropyran-type chromophore 316 (2000) 578
- Ishiuchi, S., see Mitsui, M. 317 (2000) 211
- Isoniemi, E., L. Khriachtchev, M. Pettersson and M. Räsänen, Infrared spectroscopy and 266 nm photolysis of H_2S_2 in solid Ar 311 (1999) 47
- Ito, A., T. Monobe, T. Yoshii and K. Tanaka, Electronic structures of C_{36} fulleride anions: C_{36}^- and C_{36}^{2-} 315 (1999) 348
- Ito, F. and T. Nakanaga, A jet-cooled infrared spectrum of the formic acid dimer by cavity ring-down spectroscopy 318 (2000) 571
- Ito, K., I. Tsuyumoto, A. Harata and T. Sawada, Ultrafast energy transfer of silver ultrafine particles in aqueous solutions as investigated by the ultrafast lensing effect technique 318 (2000) 1
- Ito, M., see Nakamura, M. 320 (2000) 381
- Ito, N., O. Kajimoto and K. Hara, Picosecond time-resolved fluorescence depolarization of *p*-terphenyl at high pressures 318 (2000) 118

- Ivanova, G., see Enchev, V. 314 (1999) 234
- Iwamoto, M., C.-X. Wu and O.-Y. Zhong-can, Tilting phase transition of Langmuir monolayers: a competition between steric repulsion and interaction of dipolar molecules with liquid surface 312 (1999) 7
- Iwamoto, M., see Zhao, W. 312 (1999) 572
- Iwamoto, M., see Miura, Y. 315 (1999) 1
- Iwata, S., see Satoh, K. 312 (1999) 522
- Iwata, S., see Tsurusawa, T. 315 (2000) 433
- Iwataki, T., see Mayama, H. 318 (2000) 113
- Izumi, F., see Ikeda, T. 318 (2000) 93
- Izuoka, A., see Nakazaki, J. 319 (2000) 385
- Jackson, B., see Shalashilin, D.V. 318 (2000) 305
- Jacobs, R.M.J., see Barry, H.R. 319 (2000) 125
- Jacobson, M.P. and R.W. Field, Visualizing intramolecular vibrational redistribution: expectation values of resonance operators 320 (2000) 553
- Jacon, M., see Tyuterev, V.I.G. 316 (2000) 271
- Jacquemin, D., B. Champagne and C. Hättig, Correlated frequency-dependent electronic first hyperpolarizability of small push-pull conjugated chains 319 (2000) 327
- Jäger, E.-G., see Müller, B.R. 319 (2000) 368
- Jakobsen, H.J., see Rasmussen, J.T. 314 (1999) 239
- Jana, S. and R.K. Mukherjee, Zeeman spectroscopy of Nd^{3+} ions in CsCdCl_3 crystal 320 (2000) 289
- Janda, K.C., see Seong, J. 314 (1999) 501
- Janek, J., see Luerßen, B. 316 (2000) 331
- Jankowski, K., I. Grabowski, K. Kowalski and A.J. Sadlej, A perturbative approach to the almost-linear coupled-cluster formalism 311 (1999) 265
- Janot, J.M., see Konstantaki, M. 318 (2000) 488
- Jansen, G., see Heßelmann, A. 315 (1999) 248
- Janssen, M.H.M., see Teule, J.M. 320 (2000) 177
- Jaouen, M., see Cabioc'h, T. 320 (2000) 202
- Jaramillo, J. and G.E. Scuseria, Performance of a kinetic energy density-dependent functional (VSXC) for predicting vibrational frequencies 312 (1999) 269
- Jarrell, H.C. and D. Siminovitch, Reintroduction of the quadrupolar interaction under magic-angle spinning NMR 314 (1999) 421
- Jarrold, M.F., see Shvartsburg, A.A. 317 (2000) 617
- Jarvis, G.K., D.P. Secombe and R.P. Tuckett, The effects of isotopomers in the state-selected photofragmentation of BCl_3^+ , PCl_3^+ and PBr_3^+ 315 (1999) 287
- Jarvis, G.K., C.A. Mayhew, R.Y.L. Chim, R.A. Kennedy and R.P. Tuckett, Fragmentation of the valence electronic states of SeF_6^+ and TeF_6^+ studied by threshold photoelectron-photoion coincidence spectroscopy 320 (2000) 104
- Jarvis, S.P., see Lantz, M.A. 315 (1999) 61
- Jasierski, M., see Maruszewski, K. 314 (1999) 83
- Jasny, J., see Sepiół, J. 311 (1999) 29
- Jastrzębski, W., see Kowalczyk, P. 314 (1999) 47
- Jaszewski, A.R., J. Jezierska and A. Jezierski, Hybrid density functional approach to the structures and EPR parameters of σ -type iminoxy radicals: the case of 3-oxobutan-2-iminoxyl 319 (2000) 611
- Jávorfí, T., see Osuka, A. 313 (1999) 499

- Jay-Gerin, J.-P. and C. Ferradini, A new estimate of the $\cdot\text{OH}$ radical yield at early times in the radiolysis of liquid water 317 (2000) 388
- Jeannin, C., M.T. Portella-Oberli, S. Jimenez, F. Vigliotti, B. Lang and M. Chergui, Femtosecond dynamics of electronic 'bubbles' in solid argon: viewing the inertial response and the bath coherences 316 (2000) 51
- Jedlovsky, P., M. Mezei and R. Vallauri, A molecular level explanation of the density maximum of liquid water from computer simulations with a polarizable potential model 318 (2000) 155
- Jena, P., see Gutsev, G.L. 312 (1999) 598
- Jenkins, S. and I. Morrison, The chemical character of the intermolecular bonds of seven phases of ice as revealed by ab initio calculation of electron densities 317 (2000) 97
- Jenkins, S.J. and D.A. King, Adsorbate/substrate bonding in $\text{Co}\{10\bar{1}0\}/\text{K-c}(2 \times 2)$ elucidated through first-principles theory 317 (2000) 372
- Jenkins, S.J. and D.A. King, Pentaprismene and hypostrophene from first-principles, with plane waves 317 (2000) 381
- Jenneskens, L.W., see Sarobe, M. 313 (1999) 31
- Jensen, F., see Christensen, K.Aa. 317 (2000) 400
- Jensen, J.H., see Kairys, V. 315 (1999) 140
- Jensen, P., see Tyuterev, V.I.G. 316 (2000) 271
- Jensen, P., see Osmann, G. 318 (2000) 597
- Jensen, P., see Bludský, O. 318 (2000) 607
- Jeong, G.-R., see Li, Z. 320 (2000) 70
- Jezierska, J., see Jaszewski, A.R. 319 (2000) 611
- Jezierski, A., see Jaszewski, A.R. 319 (2000) 611
- Ji, W., see Jin, Z. 318 (2000) 505
- Ji, Z. and G. Wu, Classification of the highly excited vibrational eigenstates by the nominal quantum numbers retrieved from the zero-order states: the diabatic correlation technique 311 (1999) 467
- Ji, Z. and G. Wu, Action localization and resonance of highly excited vibrational triatomic system 319 (2000) 45
- Jia, C.C., see Chen, X.J. 319 (2000) 76
- Jiang, H. and X.S. Zhao, Proposals for the propagation of quantum time-dependent self-consistent field equations 319 (2000) 555
- Jiang, M.-H., see Wu, L.-Z. 315 (1999) 379
- Jiang, Y., see Wu, J. 311 (1999) 315
- Jimenez, S., see Jeannin, C. 316 (2000) 51
- Jin, B., H.L. Schmider and D. Wardlaw, Potential energy surfaces for the collinear H_3^+ system 317 (2000) 464
- Jin, B.-Y., see Hsu, C.-C. 311 (1999) 355
- Jin, Y.D., J.P. Yang, P.L. Heremans, M. Van der Auweraer, E. Rousseau, H.J. Geise and G. Borghs, Single-layer organic light-emitting diode with 2.0% external quantum efficiency prepared by spin-coating 320 (2000) 387
- Jin, Z., X. Sun, G. Xu, S.H. Goh and W. Ji, Nonlinear optical properties of some polymer/multi-walled carbon nanotube composites 318 (2000) 505
- Jinguji, M., see Guderian, A. 312 (1999) 440
- Johnson, M.A., see Ayotte, P. 316 (2000) 455
- Johnson, M.L., see Kušba, J. 319 (2000) 661
- Johnson, P.M., see Hofstein, J.D. 316 (2000) 229
- Johnston, R.L., see Lanning, O.J. 317 (2000) 296
- Jolicard, G., see Zenevich, V.A. 312 (1999) 530

- Jolkkonen, S., see Khriachtchev, L. 316 (2000) 115
- Jones, D.E., see Rakhimov, R.R. 319 (2000) 639
- Jones, M., see Bridgeman, A.J. 314 (1999) 176
- Jones, R.H., L.H. Doerrer, S.J. Teat and C.C. Wilson, Variable-temperature diffraction study of the barrier to rotation and zero-point motion in bis(η^6 -benzene)chromium 319 (2000) 423
- Jones, T.S., see Eggeling, J. 313 (1999) 805
- Jones II, G., see Horng, M.L. 315 (1999) 363
- Joos, S., see Achatz, U. 320 (2000) 53
- Jörg, T., see Böhmer, R. 316 (2000) 419
- Jørgensen, P., see Bak, K.L. 317 (2000) 116
- Jørgensen, P., see Bak, K.L. 319 (2000) 563
- Joseph, Y., C. Kuhrs, W. Ranke, M. Ritter and W. Weiss, Adsorption of water on FeO(111) and Fe₃O₄(111): identification of active sites for dissociation 314 (1999) 195
- Jouguelet, E., C. Mathis and P. Petit, Controlling the electronic properties of single-wall carbon nanotubes by chemical doping 318 (2000) 561
- Journet, C., see Vivien, L. 312 (1999) 617
- Juanes-Marcos, J.C. and A. García-Vela, Preparation and probing of Ar–Cl radical complexes from UV photodissociation of the Ar–HCl cluster 317 (2000) 59
- Juha, L., B. Ehrenberg, S. Couris, E. Koudoumas, V. Hamplová, Z. Pokorná, A. Müllerová and M. Pavel, Fullerene decomposition induced by near-infrared laser radiation studied by real-time turbidimetry 313 (1999) 431
- Jungwirth, P., see Knospe, O. 317 (2000) 531
- Kachanov, A., see Booth, J.P. 317 (2000) 633
- Kahn, A., see Hill, I.G. 317 (2000) 444
- Kahn, O., see Létard, J.-F. 313 (1999) 115
- Kain, J.S., O.L. Polyansky and J. Tennyson, The ground-state potential energy surface of water: barrier to linearity and its effect on the vibration–rotation levels 317 (2000) 365
- Kain, J.S., see Császár, A.G. 312 (1999) 613
- Kairys, V. and J.H. Jensen, Evaluation of the charge penetration energy between non-orthogonal molecular orbitals using the Spherical Gaussian Overlap approximation 315 (1999) 140
- Kais, S., see Serra, P. 319 (2000) 273
- Kaiser, L.G., see Bush, S.D. 311 (1999) 379
- Kajimoto, O., see Ito, N. 318 (2000) 118
- Kaldor, U., see Landau, A. 313 (1999) 399
- Kalinowski, J., see Giro, G. 318 (2000) 137
- Kállay, M. and P.R. Surján, Improving CISD calculations by geminal-type reference states 312 (1999) 221
- Kaltsayannis, N. and S.D. Price, Computational studies of the geometric and electronic structures of BF₃⁺, AlF₃⁺, CF₃²⁺ and SiF₃²⁺ 313 (1999) 679
- Kamariotis, A., T. Hayes, D. Bellert and P.J. Brucat, The ground and charge-transfer excited states of CoO⁺ 316 (2000) 60
- Kameda, T., see Nakazawa, Y. 311 (1999) 362
- Kaminuma, T., see Nakano, T. 318 (2000) 614
- Kamiya, M., see Kobayashi, Y. 319 (2000) 695
- Kamiyama, T., see Ikeda, T. 318 (2000) 93
- Kanada, Y., see Tsuchida, E. 311 (1999) 236
- Kanayama, T., see Robinson, A.P.G. 312 (1999) 469
- Kanbara, T., see Inoue, T. 316 (2000) 381

- Kaneko, K., see Ohkubo, T. 312 (1999) 191
- Kanhere, D.G., see Majumder, C. 311 (1999) 62
- Karadakov, P.B. and K. Morokuma, ONIOM as an efficient tool for calculating NMR chemical shielding constants in large molecules 317 (2000) 591
- Karafiloglou, P., Quasi-linear dependence of one- and two- electron densities in natural bond orbitals 315 (1999) 446
- Karelson, M., see Yamamoto, S. 318 (2000) 590
- Karis, O., see Föhlich, A. 315 (1999) 194
- Kariuki, B.M., see Lanning, O.J. 317 (2000) 296
- Karpen, A., The intermolecular interaction in the charge-transfer complex between NH_3 and F_2 . A subtle case 316 (2000) 483
- Karplus, M., see Elber, R. 311 (1999) 335
- Kasai, T., see Ohoyama, H. 313 (1999) 484
- Kasha, M., see Catalán, J. 318 (2000) 629
- Kashevarova, L.S., see Senyavin, V.M. 313 (1999) 421
- Kashino, S., see Inoue, T. 316 (2000) 381
- Kast, S.M., see Müller, M. 311 (1999) 485
- Katada, M., see Akiyama, K. 317 (2000) 490
- Kato, N., K. Saito, H. Aida and Y. Uesu, Observations of merocyanine J-aggregate domains in mixed molecular monolayers using SHG/fluorescence and atomic force microscopes 312 (1999) 115
- Kato, T., see Akasaka, T. 319 (2000) 153
- Katrusiak, A., see Szafranski, M. 318 (2000) 427
- Kawabata, H., see Ohta, N. 315 (1999) 151
- Kawada, Y., see Nakazaki, J. 319 (2000) 385
- Kawaguchi, H., see Ohoyama, H. 313 (1999) 484
- Kawahara, S., see Uchimar, T. 318 (2000) 203
- Kawai, A., R. Kohno, N. Oki and K. Obi, Exciplex formation reaction in benzaldehyde-1,4-dimethoxybenzene clusters 318 (2000) 85
- Kawakami, T., see Shigeta, Y. 315 (1999) 441
- Kawamura, Y., see Nakai, H. 318 (2000) 298
- Kawashima, Y., Y. Ohshima and Y. Endo, Rotational spectrum of the $\text{N}_2 \cdot \cdot \text{CO}$ complex: ortho- N_2 and para- N_2 315 (1999) 201
- Kawata, M. and M. Mikami, Acceleration of the canonical molecular dynamics simulation by the particle mesh Ewald method combined with the multiple time-step integrator algorithm 313 (1999) 261
- Kawata, M. and M. Mikami, Corrigendum to "Acceleration of the canonical molecular dynamics simulation by the particle mesh Ewald method combined with the multiple time-step integrator algorithm". [Chem. Phys. Lett. 313 (1999) 261-266] 317 (2000) 515
- Kawata, S., see Ishitobi, H. 316 (2000) 578
- Kawato, S., see Shimizu, S. 317 (2000) 611
- Kawazoe, Y., see Belosludov, R.V. 312 (1999) 299
- Kawazoe, Y., see Onoe, J. 315 (1999) 19
- Ke, X.Z., Z.Y. Zhu, F.S. Zhang, F. Wang and Z.X. Wang, Molecular dynamics simulation of C_{20} fullerene 313 (1999) 40
- Kędzierski, P., see Grembecka, J. 313 (1999) 385
- Keller, C., see Föhlich, A. 315 (1999) 194
- Kelley, A.M., see Verdal, N. 320 (2000) 95

- Kelley, J.A., see Ayotte, P. 316 (2000) 455
- Kellö, V., P. Pykkö, A.J. Sadlej, P. Schwerdtfeger and J. Thyssen, The nuclear quadrupole moment of ^{91}Zr from molecular data for ZrO and ZrS 318 (2000) 222
- Kellö, V., K.P. Lawley and G.H.F. Dierksen, An ab initio Investigation of the dipole moment of the $\text{CO}_2 \cdots \text{CO}$ complex 319 (2000) 231
- Kelly, K.F., I.W. Chiang, E.T. Mickelson, R.H. Hauge, J.L. Margrave, X. Wang, G.E. Scuseria, C. Radloff and N.J. Halas, Insight into the mechanism of sidewall functionalization of single-walled nanotubes: an STM study 313 (1999) 445
- Kemp-Harper, R., see McManus, J. 311 (1999) 292
- Kempgens, B., see Neeb, M. 320 (2000) 217
- Kennedy, R.A., see Jarvis, G.K. 320 (2000) 104
- Kennedy, S.D., see Chen, Z. 313 (1999) 217
- Keuleers, R., see Miao, M.S. 316 (2000) 297
- Khait, Y.G., see Hoffmann, M.R. 311 (1999) 372
- Khamaganov, V.I., see Richter, R.C. 319 (2000) 341
- Khan, A., Ab initio studies of $(\text{H}_2\text{O})_{20}\text{H}^+$ and $(\text{H}_2\text{O})_{21}\text{H}^+$ prismatic, fused cubic and dodecahedral clusters: can H_3O^+ ion remain in cage cavity? 319 (2000) 440
- Kharlanov, V., see Rettig, W. 318 (2000) 173
- Khriachtchev, L., M. Pettersson, S. Jolkkonen and M. Räsänen, UV photolysis in rare-gas solids: spectral overlap between absorbers and emitters 316 (2000) 115
- Khriachtchev, L., see Isoniemi, E. 311 (1999) 47
- Kiefer, B., see Rubner, O. 316 (2000) 585
- Kiefer, W., see Vierheilig, A. 312 (1999) 349
- Kierzkowski, P., see Pranszke, B. 317 (2000) 220
- Kikuchi, K., K. Akiyama, K. Sakaguchi, T. Kodama, H. Nishikawa, I. Ikemoto, T. Ishigaki, Y. Achiba, K. Sueki and H. Nakahara, Production and isolation of the isomers of dimetallofullerenes, HoTm@C_{82} and $\text{Tm}_2\text{@C}_{82}$ 319 (2000) 472
- Kikuchi, K., see Akiyama, K. 317 (2000) 490
- Kikuchi, K., see Washizu, H. 320 (2000) 277
- Kim, C.K., see Lee, I. 320 (2000) 307
- Kim, D.W., see Lee, C.J. 312 (1999) 461
- Kim, H.-S., A Monte Carlo simulation study of the solvent effect on the relative free energies of solvation and the partition coefficients of organic solutes 317 (2000) 555
- Kim, H.S., see Shin, Y.B. 317 (2000) 639
- Kim, J., see Vijaya Sarathy, K. 318 (2000) 543
- Kim, J.M., see Lee, C.J. 312 (1999) 461
- Kim, J.S., P.K.H. Ho, D.S. Thomas, R.H. Friend, F. Cacialli, G.-W. Bao and S.F.Y. Li, X-ray photoelectron spectroscopy of surface-treated indium-tin oxide thin films 315 (1999) 307
- Kim, S.Y., G.Y. Lee, S.Y. Han and M. Lee, Fluorescence quenching dynamics of azulene and 2-haloazulenes by CCl_4 in nonpolar solvents 318 (2000) 63
- Kim, Y., K. Patton, J. Fleniken and H. Meyer, Rotationally resolved overtone spectroscopy of the NO-Ar complex 318 (2000) 522
- Kim, Y., see Christoffel, K.M. 315 (1999) 275
- Kim, Y., see Fleniken, J. 318 (2000) 529
- Kim, Y.-K., see Huo, W.M. 319 (2000) 576
- Kim, Y.H., J. Ree and H.K. Shin, Formation of vibrationally excited hydrogen molecules on a graphite surface 314 (1999) 1
- Kimmich, R., see Ardelean, I. 320 (2000) 81

- Kimura, S., see Miura, Y. 315 (1999) 1
- King, D.A., see Kose, R. 311 (1999) 109
- King, D.A., see Kose, R. 313 (1999) 1
- King, D.A., see Arnolds, H. 314 (1999) 389
- King, D.A., see Jenkins, S.J. 317 (2000) 372
- King, D.A., see Jenkins, S.J. 317 (2000) 381
- King, G.C., see Mielewska, B. 311 (1999) 428
- King, G.C., see Yench, A.J. 315 (1999) 37
- King, K.D., see Alexander, U.N. 319 (2000) 529
- Kinoshita, M. and Y. Sugai, A new methodology for predicting shape and size distribution of micelles 313 (1999) 685
- Kippelen, B., see Golemme, A. 319 (2000) 655
- Kira, M., see Manaka, T. 317 (2000) 260
- Kirbach, U., see Fedurco, M. 319 (2000) 309
- Kiskinova, M., see Luerßen, B. 316 (2000) 331
- Kitagawa, Y., see Soda, T. 319 (2000) 223
- Kitaura, K., T. Sawai, T. Asada, T. Nakano and M. Uebayasi, Pair interaction molecular orbital method: an approximate computational method for molecular interactions 312 (1999) 319
- Kitaura, K., E. Ikeo, T. Asada, T. Nakano and M. Uebayasi, Fragment molecular orbital method: an approximate computational method for large molecules 313 (1999) 701
- Kitaura, K., see Nakano, T. 318 (2000) 614
- Kitiyanan, B., W.E. Alvarez, J.H. Harwell and D.E. Resasco, Controlled production of single-wall carbon nanotubes by catalytic decomposition of CO on bimetallic Co-Mo catalysts 317 (2000) 497
- Kivimäki, A., see Neeb, M. 320 (2000) 217
- Klamroth, T., see Bartels, L. 313 (1999) 544
- Klee, W.E., see Winkler, B. 312 (1999) 536
- Klein, G., Transient femtosecond spectroscopy in α -sexithiophene single crystals 320 (2000) 65
- Kleine, D., S. Stry, J. Lauterbach, K. Kleinermanns and P. Hering, Measurement of the absolute intensity of the fifth CH stretching overtone of benzene using cavity ring-down spectroscopy 312 (1999) 185
- Kleinekathöfer, U., see Nest, M. 313 (1999) 665
- Kleinermanns, K., see Kleine, D. 312 (1999) 185
- Kleyn, A.W., see Ciobîcă, I.M. 311 (1999) 185
- Klimov, V.I., see Wang, H.-L. 315 (1999) 173
- Klinowski, J., see Collins, C. 312 (1999) 346
- Klinowski, J., see Gandy, P.J.F. 314 (1999) 543
- Klopper, W., see Halkier, A. 319 (2000) 287
- Klossika, J.-J., H. Flöthmann, R. Schinke and M. Bittererová, On the $S_1 \rightarrow S_0$ internal conversion in the photodissociation of HNCO 314 (1999) 182
- Klostermann, K., see Fedurco, M. 319 (2000) 309
- Knak Jensen, S.J. and I.G. Csizmadia, Strong and symmetric hydrogen bonding in the hydrogen di-superoxide anion 319 (2000) 220
- Kneip, C., P. Hildebrandt, K. Németh, F. Mark and K. Schaffner, Interpretation of the resonance Raman spectra of linear tetrapyrroles based on DFT calculations 311 (1999) 479
- Knight, A.M., see Agreiter, J.K. 313 (1999) 162
- Knight, K.S., see Carter, V.J. 313 (1999) 505

- Knochenmuss, R., Photoionization, fragmentation and proton transfer in 1-naphthol(NH₃)_n clusters 311 (1999) 439
- Knospe, O. and P. Jungwirth, Electron photodetachment in C₆₀⁻: Quantum molecular dynamics with a non-empirical, 'on-the-fly' calculated potential 317 (2000) 531
- Knowles, P.J., see Panten, D. 311 (1999) 390
- Knowles, P.J., see Manby, F.R. 312 (1999) 347
- Knupfer, M., J. Fink, E. Zojer, G. Leising and D. Fichou, Universal exciton size scaling in π conjugated systems 318 (2000) 585
- Kobayashi, K. and S. Nagase, Theoretical study of structures and dynamic properties of Sc₃@C₈₂ 313 (1999) 45
- Kobayashi, K., see Kurita, N. 313 (1999) 693
- Kobayashi, K., see Akasaka, T. 319 (2000) 153
- Kobayashi, S., see Miura, Y. 315 (1999) 1
- Kobayashi, T., see Chin, B.-C. 318 (2000) 499
- Kobayashi, Y., M. Kamiya and K. Hirao, The hydrogen abstraction reactions: a multireference Møller–Plesset perturbation (MRMP) theory study 319 (2000) 695
- Kodaira, T., see Ikeda, T. 318 (2000) 93
- Kodama, T., see Akiyama, K. 317 (2000) 490
- Kodama, T., see Kikuchi, K. 319 (2000) 472
- Koglin, E. and R.J. Meier, An ab-initio study of the relative stability of the ggg and the gtg conformer in hexane 312 (1999) 284
- Köhler, J., see Durand, Y. 317 (2000) 232
- Kohno, J.-y., see Horimoto, N. 318 (2000) 536
- Kohno, M., S. Ogura, K. Sato and Y. Inoue, A tracer study of a radical produced by UV irradiation on BaTi₄O₉ photocatalyst surface 319 (2000) 451
- Kohno, R., see Kawai, A. 318 (2000) 85
- Kohtani, S., A. Tagami and R. Nakagaki, Excited-state proton transfer of 7-hydroxyquinoline in a non-polar medium: mechanism of triple proton transfer in the hydrogen-bonded system 316 (2000) 88
- Koizumi, H., see Ichikawa, T. 313 (1999) 129
- Koizumi, H., see Fukumoto, Y. 313 (1999) 283
- Kolb, D., see Kullie, O. 314 (1999) 307
- Kolmakov, A., J.O. Löfken, C. Nowak, F. Picucci, M. Riedler, C. Rienecker, A. Wark, M. Wolff and T. Möller, Argon coated alkali halide clusters: the effect of the coating on the ionization and fragmentation dynamics 319 (2000) 465
- Kołos, R., see Sepiol, J. 311 (1999) 29
- Komaguchi, K., see Wang, P. 320 (2000) 623
- Komasa, J., see Cioslowski, J. 319 (2000) 542
- Konarev, D.V., R.N. Lyubovskaya, N.V. Drichko, V.N. Semkin and A. Graja, Energies of charge transfer for C₆₀ and C₇₀ complexes in solutions and in the solid state 314 (1999) 570
- Konarev, D.V., see Steinman, E.A. 319 (2000) 1
- Kondo, M., see Akasaka, T. 319 (2000) 153
- Kondow, T., see Horimoto, N. 318 (2000) 536
- Kong, W., see Castle, K.J. 318 (2000) 565
- Konstantaki, M., E. Koudoumas, S. Couris, J.M. Janot, H. Eddaoudi, A. Deratani, P. Seta and S. Leach, Optical limiting behaviour of the water-soluble C₆₀/γ-cyclodextrin complex 318 (2000) 488
- Kónya, Z., see Willems, I. 317 (2000) 71

- Kónya, Z., see Colomer, J.-F. 317 (2000) 83
- Kooi, S.E. and A.W. Castleman Jr., Dehydrogenation of ammonia by early transition metals: formation of metal nitride clusters 315 (1999) 49
- Koolen, J.H., V. Moulton and I. Gutman, Improving the McClelland inequality for total π -electron energy 320 (2000) 213
320 (2000) 217
- Köppe, H.M., see Neeb, M. 320 (2000) 237
- Kopot, J., An ab initio study on the equilibrium structure and CCC bending energy levels of carbon suboxide 318 (2000) 203
- Korchowiec, J., see Uchimaru, T.
- Kose, R., W.A. Brown and D.A. King, Determination of the Rh–C bond energy for C_2H_2 and C_2H_4 reactive adsorption on Rh(100) 311 (1999) 109
- Kose, R. and D.A. King, Energetics and CO-induced lifting of a (1×2) surface reconstruction observed on Pt(311) 313 (1999) 1
313 (1999) 771
- Koshi, M., see Tonokura, K. 319 (2000) 507
- Koshi, M., see Tonokura, K. 317 (2000) 260
- Koshihara, S., see Manaka, T. 313 (1999) 155
- Kosloff, R., see Wang, Z. 311 (1999) 299
- Kosugi, N., see Pettersson, L.G.M. 320 (2000) 217
- Kosugi, N., see Neeb, M. 320 (2000) 19
- Kosyakov, V.I., see Bulgakov, A.V. 317 (2000) 611
- Kou, J., see Shimizu, S. 313 (1999) 431
- Koudoumas, E., see Juha, L. 318 (2000) 488
- Koudoumas, E., see Konstantaki, M. 319 (2000) 460
- Kouzoudis, D., see Grimes, C.A. 319 (2000) 238
- Kovács, A., Theoretical study of rare earth trihalide dimers Ln_2X_6 ($Ln = La, Dy$; $X = F, Cl, Br, I$) 320 (2000) 186
- Kovalenko, A., see Shapovalov, V.
- Kowalczyk, P., W. Jastrzębski, A. Pashov, S. Magnier and M. Aubert-Frécon, Potential energies of the $4^1\Pi$ and $5^1\Pi$ states of NaK by polarization labelling spectroscopy and by ab initio calculations 314 (1999) 47
315 (1999) 355
- Kowalski, A., see Ottinger, C. 317 (2000) 220
- Kowalski, A., see Pranszke, B. 311 (1999) 265
- Kowalski, K., see Jankowski, K. 315 (1999) 75
- Koyama, Y., see Onaka, K. 318 (2000) 597
- Kraemer, W.P., see Osmann, G. 313 (1999) 393
- Kratochvíl, M., see Ryjáček, F. 312 (1999) 440
- Kraus, M., see Guderian, A. 314 (1999) 176
- Krausz, E., see Bridgeman, A.J.
- Krawczyk, R.P., K. Malsch, G. Hohlneicher, R.C. Gillen and W. Domcke, $1^1B_u-2^1A_g$ conical intersection in *trans*-butadiene: ultrafast dynamics and optical spectra 320 (2000) 535
315 (1999) 125
- Krimm, S., see Qian, W. 311 (1999) 55
- Krishnamoorthy, G., see Santra, S. 317 (2000) 481
- Krissinel, E.B., see Frantsuzov, P.A.
- Krokidis, X., N.W. Moriarty, W.A. Lester, Jr. and M. Frenklach, Propargyl radical: an electron localization function study 314 (1999) 534
313 (1999) 725
- Król, S., see Graja, A. 317 (2000) 77
- Kroto, H.W., see Hsu, W.K. 318 (2000) 555
- Kruger, C.H., see Zhao, M.

- Kruger, C.H., see Lommatzsch, U. 320 (2000) 339
- Krupa, J.-C., see Yin, M. 314 (1999) 27
- Krupski, M., see Augustyniak, M.A. 311 (1999) 126
- Kryachko, E.S., Ab initio studies of the conformations of water hexamer: modelling the penta-coordinated hydrogen-bonded pattern in liquid water 314 (1999) 353
- Kryachko, E.S., Generalized idempotency purification transform in linear scaling self-consistent field theory 318 (2000) 210
- Ku, J.K., see Son, H.S. 320 (2000) 658
- Kubicki, J., see Bojarski, P. 318 (2000) 379
- Kubo, M., see Shrivastava, K.N. 313 (1999) 279
- Kubozono, Y., see Inoue, T. 316 (2000) 381
- Kucharski, S.A., see Musiał, M. 320 (2000) 542
- Kuczkowski, R.L., see Peebles, S.A. 312 (1999) 357
- Kudo, H., see Yokoyama, K. 320 (2000) 645
- Kuhlenbeck, H., see Wolter, K. 320 (2000) 206
- Kühnle, A., see Bartels, L. 313 (1999) 544
- Kuhrs, C., see Joseph, Y. 314 (1999) 195
- Kujanpää, J.P., see Carter, V.J. 313 (1999) 505
- Kuki, M., see Onaka, K. 315 (1999) 75
- Kukovitsky, E.F., S.G. L'vov and N.A. Sainov, VLS-growth of carbon nanotubes from the vapor 317 (2000) 65
- Kulak, L., see Bojarski, P. 318 (2000) 379
- Kullie, O., C. Düsterhöft and D. Kolb, Dirac–Fock finite element method (FEM) calculations for some diatomic molecules 314 (1999) 307
- Kulshreshtha, S.K., see Majumder, C. 311 (1999) 62
- Kumada, T., see Shevtsov, V. 319 (2000) 535
- Kumar, A., see Mahesh, T.S. 319 (2000) 278
- Kumaran, S.S., see Michael, J.V. 319 (2000) 99
- Kumar Mondal, C., P. Chaudhury and S.P. Bhattacharyya, Photo-dissociation dynamics of a diatomic molecule: modelling of thermal and environmental effects 311 (1999) 400
- Kume, T., see Osuka, A. 313 (1999) 499
- Kunkely, H. and A. Vogler, Photoluminescence of $[\text{Rh}^{\text{III}}(\text{phpy})_2(\text{CN})_2]^-$ (phpy[−] = *ortho*-metalated 2-phenylpyridine anion) 319 (2000) 486
- Kunugi, Y., see Harima, Y. 317 (2000) 310
- Kunz, M., see van Smaalen, S. 319 (2000) 283
- Kuo, C.T., see Nee, J.B. 318 (2000) 402
- Kupče, Ě., see Linden, N. 311 (1999) 321
- Küppers, J., see Dinger, A. 311 (1999) 202
- Küppers, J., see Dinger, A. 320 (2000) 405
- Kurin-Csörgei, K., M. Orbán, A.M. Zhabotinsky and I.R. Epstein, Reply to Comment on “On the nature of patterns arising during polymerization of acrylamide in the presence of the methylene blue–sulfide–oxygen oscillating reaction”. [Chem. Phys. Lett. 311 (1999) 102–104] 311 (1999) 105
- Kurita, N., M. Araki, K. Nakao and K. Kobayashi, Efficiency of the MO method using a Slater-type basis set and non-local density functional formalism for describing DNA base stacking energy 313 (1999) 693
- Kurosaki, Y., see Takayanagi, T. 312 (1999) 503
- Kurosawa, T., see Ohmori, K. 315 (1999) 411

- Kuśba, J., G. Piszczek, I. Gryczynski, M.L. Johnson and J.R. Lakowicz, Effects of diffusion on energy transfer in solution using a microsecond decay time rhenium metal-ligand complex as the donor 319 (2000) 661
- Kushida, T., see Tanaka, M. 315 (1999) 428
- Kusumi, T., see Lantz, M.A. 315 (1999) 61
- Kutznigg, W. and D. Mukherjee, Direct determination of the cumulants of the reduced density matrices 317 (2000) 569
- Kuyucak, S., see Allen, T.W. 313 (1999) 358
- Kuyucak, S., see Corry, B. 320 (2000) 35
- Kuz'menko, N.E., see Eryomin, V.V. 316 (2000) 303
- Kveder, V.V., see Steinman, E.A. 319 (2000) 1
- Kwon, O., M.L. McKee and R.M. Metzger, Theoretical calculations of methylquinolinium tricyanoquinodimethanide ($\text{CH}_3\text{Q}-3\text{CNQ}$) using a solvation model 313 (1999) 321
- Kwong, H.L., see Zhang, X.H. 320 (2000) 77
- Laaksonen, A., see Uličný, J. 319 (2000) 396
- Labazan, I., S. Rudić and S. Milošević, Nonlinear effects in pulsed cavity ringdown spectroscopy of lithium vapour 320 (2000) 613
- Ladik, J., see Hu, A. 320 (2000) 6
- Laenen, R., see Assel, M. 317 (2000) 13
- Lafonta, F., see Vivien, L. 312 (1999) 617
- Laganà, A., see Alvarino, J.M. 313 (1999) 299
- Lahiri, A. and L. Nilsson, Examining the characteristics of chaos in biomolecular dynamics: a random matrix approximation 311 (1999) 459
- Lai, H.L., see Zhou, X.T. 318 (2000) 58
- Lai, M.Y., see Mebel, A.M. 318 (2000) 27
- Lai, W.Y., see Cheng, L.F. 319 (2000) 418
- Lai, W.Y., see Zhang, X.H. 320 (2000) 77
- Lakowicz, J.R., see Kuśba, J. 319 (2000) 661
- La Manna, G., see Cottone, G. 319 (2000) 51
- Lamb, D.W. and G.L.D. Ritchie, Erratum to "Cotton-Mouton effect, magnetizability anisotropy and molecular charge distribution of boron trichloride". [Chem. Phys. Lett. 310 (1999) 150-154] 317 (2000) 655
- Landau, A., E. Eliav and U. Kaldor, Intermediate Hamiltonian Fock-space coupled-cluster method 313 (1999) 399
- Lang, B., see Jeannin, C. 316 (2000) 51
- Langenberg, J.D., see Fabbi, J.C. 320 (2000) 303
- Langenscheidt, A., see Gödicke, B. 318 (2000) 102
- Lanning, O.J., S. Habershon, K.D.M. Harris, R.L. Johnston, B.M. Kariuki, E. Tedesco and G.W. Turner, Definition of a 'guiding function' in global optimization: a hybrid approach combining energy and *R*-factor in structure solution from powder diffraction data 317 (2000) 296
- Lantz, M.A., S.P. Jarvis, H. Tokumoto, T. Martynski, T. Kusumi, C. Nakamura and J. Miyake, Stretching the α -helix: a direct measure of the hydrogen-bond energy of a single-peptide molecule 315 (1999) 61
- Lanzani, G., S. Stagira, G. Cerullo, S. De Silvestri, D. Comoretto, I. Moggio, C. Cuniberti, G.F. Musso and G. Dellepiane, Triplet exciton generation and decay in a red polydiacetylene studied by femtosecond spectroscopy 313 (1999) 525

- Lapersonne-Meyer, C., see Lécuyer, R. 314 (1999) 255
- Laplaze, D., see Alvarez, L. 316 (2000) 186
- Largent, C.C., see Zhao, M. 318 (2000) 555
- Largo, A., see Redondo, P. 315 (1999) 224
- Largo, A., see Barrientos, C. 320 (2000) 481
- Laroche, M., M. Bettinelli, S. Girard and R. Moncorgé, f-d Luminescence of Pr^{3+} and Ce^{3+} in the chloro-elpasolite $\text{Cs}_2\text{NaYCl}_6$ 311 (1999) 167
- Lascoux, N., see Gale, G.M. 311 (1999) 123
- Latajka, Z., see Biczysko, M. 313 (1999) 366
- Latini, A., see Satta, M. 316 (2000) 94
- Latychevskaia, T., see Sepiol, J. 311 (1999) 29
- Lau, J.T., A. Achleitner and W. Wurth, X-ray absorption spectroscopy of size-selected, deposited small chromium clusters 317 (2000) 269
- Lau, K.-C., see Ma, N.L. 311 (1999) 275
- Lau, K.H., see Hildenbrand, D.L. 319 (2000) 95
- Laubereau, A., see Saß, M. 311 (1999) 13
- Laubereau, A., see Assel, M. 317 (2000) 13
- Laurent, Ch., see Colomer, J.-F. 317 (2000) 83
- Lauterbach, J., see Kleine, D. 312 (1999) 185
- Lavendy, H., see Pascoli, G. 312 (1999) 333
- Lawler, J.E., see Peck, J.R. 318 (2000) 476
- Lawley, K.P., see Kellö, V. 319 (2000) 231
- Lawrance, W.D., see Alexander, U.N. 319 (2000) 529
- Laxmikanth Rao, J., see Bhanuprakash, K. 314 (1999) 282
- Leach, S., see Konstantaki, M. 318 (2000) 488
- Leard, D.C., see Lee, S.-H. 315 (1999) 7
- Leclerc, M., see Belletête, M. 316 (2000) 101
- Lécuyer, R., J. Berréhar, C. Lapersonne-Meyer, M. Schott and J.-D. Ganière, Fluorescence quantum yield and lifetime of 'red' polydiacetylene chains isolated in their crystalline monomer matrix 314 (1999) 255
- Lee, A.M. and P.M.W. Gill, Computation of Coulomb and exchange radial intracule densities 313 (1999) 271
- Lee, B.-S., see Lee, I. 320 (2000) 307
- Lee, C.J., D.W. Kim, T.J. Lee, Y.C. Choi, Y.S. Park, Y.H. Lee, W.B. Choi, N.S. Lee, G.-S. Park and J.M. Kim, Synthesis of aligned carbon nanotubes using thermal chemical vapor deposition 312 (1999) 461
- Lee, C.S., see Tang, Y.H. 314 (1999) 16
- Lee, C.S., see Zhou, X.T. 318 (2000) 58
- Lee, C.S., see Cheng, L.F. 319 (2000) 418
- Lee, C.S., see Zhang, X.H. 320 (2000) 77
- Lee, C.W., K.S. Wong, J.D. Huang, S.V. Frolov and Z.V. Vardeny, Femtosecond time-resolved laser action in poly(*p*-phenylene vinylene) films: stimulated emission in an inhomogeneously broadened exciton distribution 314 (1999) 564
- Lee, E.P.F. and T.G. Wright, $\text{NO}^+\cdot\text{O}_2$ versus NO_3^+ - which is the more stable? 318 (2000) 196
- Lee, E.P.F., see Soldán, P. 313 (1999) 379
- Lee, G.Y., see Kim, S.Y. 318 (2000) 63
- Lee, H.W., see Lee, I. 320 (2000) 307

- Lee, I., C.K. Kim, H.G. Li, B.-S. Lee and H.W. Lee, Inversion of stationary point levels in a flat transition structure region on account of vibrational energy 320 (2000) 307
- Lee, K., see Son, H.S. 320 (2000) 658
- Lee, M., see Kim, S.Y. 318 (2000) 63
- Lee, M.S., see Maslen, P.E. 319 (2000) 205
- Lee, N.S., see Lee, C.J. 312 (1999) 461
- Lee, S.-H., D.C. Leard, R. Zhang, L.T. Molina and M.J. Molina, The $\text{HCl} + \text{ClONO}_2$ reaction rate on various water ice surfaces 315 (1999) 7
- Lee, S.-H. and K. Liu, Erratum to: "Isotope effects and excitation functions for the reactions of $\text{S}(^1\text{D}) + \text{H}_2$, D_2 and HD [Chem. Phys. Lett. 290 (1998) 323]" 317 (2000) 516
- Lee, S.-L., see Mishra, R.K. 313 (1999) 437
- Lee, S.K. and D.Y. Baek, Visible vibronic emission spectrum of the jet-cooled pentafluorobenzyl radical 311 (1999) 36
- Lee, S.K. and B.U. Ahn, Vibronic spectroscopy of jet-cooled *p*-cyanobenzyl radical: $\text{D}_1 \rightarrow \text{D}_0$ spectra and vibrational mode assignments 320 (2000) 601
- Lee, S.T., see Tang, Y.H. 314 (1999) 16
- Lee, S.T., see Zhou, X.T. 318 (2000) 58
- Lee, S.T., see Zhang, R.Q. 319 (2000) 213
- Lee, S.T., see Cheng, L.F. 319 (2000) 418
- Lee, S.T., see Zhang, X.H. 320 (2000) 77
- Lee, T.J., see Lee, C.J. 312 (1999) 461
- Lee, Y.H., see Lee, C.J. 312 (1999) 461
- Lee, Y.Z., see Chang, R. 317 (2000) 153
- Lefrant, S., see Colomer, J.-F. 317 (2000) 83
- Legay, F., see Legay-Sommaire, N. 314 (1999) 40
- Legay-Sommaire, N. and F. Legay, Photochemical insertion of Hg in the HCl bond and mercury-sensitized production of ClHCl^- and KrHKr^+ in low-temperature matrices 314 (1999) 40
- Le Goff, G., see Berthault, P. 314 (1999) 52
- Legon, A.C. and E.R. Waclawik, Angular geometry, binding strength and charge transfer for the complex $\text{H}_2\text{S} \cdots \text{ICl}$ determined by rotational spectroscopy 312 (1999) 385
- Legon, A.C., Angular and radial geometries, charge transfer and binding strength in isolated complexes $\text{B} \cdots \text{ICl}$: some generalisations 314 (1999) 472
- Legon, A.C., see McIntosh, A. 314 (1999) 57
- Leibeling, G., see Müller, B.R. 319 (2000) 368
- Leibl, W., see Gibasiewicz, K. 315 (1999) 95
- Leising, G., see Ariu, M. 313 (1999) 405
- Leising, G., see Knupfer, M. 318 (2000) 585
- Leite, V.B.P., M. Ferreira and O.N. Oliveira Jr., Electron transfer between adjacent layers in self-assembled films 316 (2000) 343
- Leiva, E.P.M., M.G. Del Pópolo and W. Schmickler, Changes in surface stress caused by the adsorption of an epitaxial metal monolayer 320 (2000) 393
- Lemoine, D., Optimized grid representations in curvilinear coordinates: the mapped sine Fourier method 320 (2000) 492
- Lentz, D., see Huckauf, A. 319 (2000) 265
- Leone, S.R., see Li, J. 313 (1999) 76
- Leonhardt, M., O. Mager and H. Port, Two-component optical spectra in thin PTCDA films due to the coexistence of α - and β -phase 313 (1999) 24
- Lesage, A., see Sakellariou, D. 319 (2000) 253

- Lesclaux, R., see Tomas, A. 319 (2000) 521
- Leskiw, B.D. and A.W. Castleman Jr., The interplay between the electronic structure and reactivity of aluminum clusters: model systems as building blocks for cluster assembled materials 316 (2000) 31
- Lester, Jr., W.A., see Krokidis, X. 314 (1999) 534
- Leszczynski, J., see Gu, J. 311 (1999) 209
- Leszczynski, J., see Roszak, S. 313 (1999) 198
- Leszczynski, J., see Roszak, S. 314 (1999) 333
- Leszczynski, J., see Pelmenchikov, A. 314 (1999) 496
- Létard, J.-F., L. Capes, G. Chastanet, N. Moliner, S. Létard, J.-A. Real and O. Kahn, Critical temperature of the LIESST effect in iron(II) spin crossover compounds 313 (1999) 115
- Létard, S., see Létard, J.-F. 313 (1999) 115
- Letokhov, V.S., see Dem'yanenko, A.V. 320 (2000) 594
- Lettenberger, M., see Saß, M. 311 (1999) 13
- Leupold, D., see Fiedor, L. 319 (2000) 145
- Levin, P.P. and S.M.B. Costa, Kinetics of oxygen induced delayed fluorescence of eosin adsorbed on alumina. The dependence on dye and oxygen concentrations 320 (2000) 194
- Levinger, N.E., see Elles, C.G. 317 (2000) 626
- Levis, R.J., see Arnolds, H. 314 (1999) 389
- Li, C., see Suo, Z. 315 (1999) 321
- Li, D.-C., L. Dai, S. Huang, A.W.H. Mau and Z.L. Wang, Structure and growth of aligned carbon nanotube films by pyrolysis 316 (2000) 349
- Li, G., see Zhang, N. 313 (1999) 69
- Li, G.-L., see Xu, W.-G. 314 (1999) 300
- Li, G.Q., see Deng, J.K. 313 (1999) 134
- Li, H., see Liu, B. 320 (2000) 365
- Li, H.G., see Lee, I. 320 (2000) 307
- Li, J., V.M. Bierbaum and S.R. Leone, Laser ionization time-of-flight mass spectrometer detection of methyl radical produced by ion-molecule reactions in a flowing-afterglow apparatus 313 (1999) 76
- Li, J., see Feng, S. 316 (2000) 146
- Li, J., see Chen, X.L. 318 (2000) 107
- Li, L., see Wang, F. 316 (2000) 318
- Li, L., see Chen, X.L. 318 (2000) 107
- Li, Q. and L. Luo, Adsorption kinetics in the solution of a thermal hysteresis protein 320 (2000) 335
- Li, Q.-S., see Xu, W.-G. 314 (1999) 300
- Li, S., see Xu, W.-G. 314 (1999) 300
- Li, S.-M., see Yu, X. 320 (2000) 123
- Li, S.F.Y., see Kim, J.S. 315 (1999) 307
- Li, T. and P.B. Balbuena, Theoretical studies of the reduction of ethylene carbonate 317 (2000) 421
- Li, W.-H., X.-Y. Li and N.-T. Yu, Surface-enhanced resonance hyper-Raman scattering and surface-enhanced resonance Raman scattering of dyes adsorbed on silver electrode and silver colloid: a comparison study 312 (1999) 28
- Li, W.-K., see Ma, N.L. 311 (1999) 275
- Li, W.Z., see Hsu, W.K. 317 (2000) 77
- Li, X.-Y., see Li, W.-H. 312 (1999) 28
- Li, Y., see Good, D.A. 313 (1999) 267
- Li, Y., see Hansen, J.C. 314 (1999) 341

- Li, Z., A. Chou and F.-M. Tao, Ab initio study of the intermolecular potential surface of He-NH₃ 313 (1999) 313
- Li, Z., G.-R. Jeong, J.C. Hansen, D.A. Good and J.S. Francisco, Rate constant for the reactions of CF₃OCHFCF₃ with OH and Cl 320 (2000) 70
- Li, Z., see Hansen, J.C. 314 (1999) 341
- Li, Z.-Q., see Belosludov, R.V. 312 (1999) 299
- Li, Z.-S., see Yu, X. 320 (2000) 123
- Lian, Y., see Okazaki, T. 320 (2000) 435
- Liang, F., see Zhang, D. 317 (2000) 430
- Liang, K.K., see Chang, R. 317 (2000) 142
- Liang, Y., see Du, X. 313 (1999) 565
- Liao, L.S., see Zhou, X.T. 318 (2000) 58
- Liao, L.S., see Cheng, L.F. 319 (2000) 418
- Lichanot, A., R. Orlando, G. Mallia, M. Mérawa and R. Dovesi, V_{OH} center in magnesium oxide: an ab initio supercell study 318 (2000) 240
- Lievens, P., see Bouwen, W. 314 (1999) 227
- Lifshitz, C., see Zhu, C. 320 (2000) 513
- Lim, K.H. and C.P. Grey, Triple quantum cross-polarization NMR of ¹H/²⁷Al and ¹⁹F/²³Na spin systems in solids 312 (1999) 45
- Lim, K.P., see Michael, J.V. 319 (2000) 99
- Lima, J.C., see Osuka, A. 313 (1999) 499
- Lin, L., see Qian, W. 319 (2000) 89
- Lin, M.-S., see Wei, T.-H. 318 (2000) 53
- Lin, S.H., see Chang, R. 317 (2000) 142
- Lin, S.H., see Chang, R. 317 (2000) 153
- Lin, S.H., see Chang, A.H.H. 320 (2000) 161
- Lin, W.F., M.S. Zei and G. Ertl, Identification of the structure of a CO adlayer on a Pt(111) electrode 312 (1999) 1
- Lin, Y., see Qian, W. 319 (2000) 89
- Lin, Y.-T., see Mishra, R.K. 313 (1999) 437
- Linden, N., Ē. Kupče and R. Freeman, NMR quantum logic gates for homonuclear spin systems 311 (1999) 321
- Lineberger, W.C., see Sanov, A. 313 (1999) 812
- Link, S., C. Burda, B. Nikoobakht and M.A. El-Sayed, How long does it take to melt a gold nanorod? A femtosecond pump-probe absorption spectroscopic study 315 (1999) 12
- Link, S., see Mohamed, M.B. 317 (2000) 519
- Linnartz, H., see Pflüger, D. 313 (1999) 171
- Lipiec, R., see Graja, A. 313 (1999) 725
- Litorja, M., see Ruscic, B. 316 (2000) 45
- Litvinchuk, A.P., see Iliev, M.N. 316 (2000) 217
- Liu, B., T. Wågberg, E. Olsson, R. Yang, H. Li, S. Zhang, H. Yang, G. Zou and B. Sundqvist, Synthesis and characterization of single-walled nanotubes produced with Ce/Ni as catalysts 320 (2000) 365
- Liu, C., see Zhang, D. 317 (2000) 430
- Liu, C., see Bu, Y. 319 (2000) 725
- Liu, C.B., see Lu, W.C. 311 (1999) 491
- Liu, D., W.-H. Fang and X.-Y. Fu, Ab initio molecular orbital study of the mechanism of photodissociation of formamide 318 (2000) 291

- Liu, G., see Cioslowski, J. 316 (2000) 536
- Liu, G., see Cioslowski, J. 319 (2000) 542
- Liu, H., see Liu, Y. 317 (2000) 181
- Liu, J.-Y., see Yu, X. 320 (2000) 123
- Liu, K., see Lee, S.-H. 317 (2000) 516
- Liu, Q.P., see Zou, Z. 312 (1999) 149
- Liu, R., see Ignatyev, I.S. 320 (2000) 469
- Liu, S., see Hsu, C.-C. 311 (1999) 355
- Liu, T., see Guo, L. 318 (2000) 49
- Liu, T.-T., see Wei, T.-X. 319 (2000) 7
- Liu, X., see Lu, Q. 314 (1999) 37
- Liu, X., see Dai, Z. 317 (2000) 9
- Liu, Y., H. Liu, H. Gao, C. Duan, P.A. Hamilton and P.B. Davies, Near-infrared laser absorption spectroscopy of the CS^+ cation 317 (2000) 181
- Liu, Y.M., see Chen, X.L. 318 (2000) 107
- Liu, Z.F., C.K. Siu and J.S. Tse, Ab initio molecular dynamics study on the hydrolysis of molecular chlorine 311 (1999) 93
- Liu, Z.F., C.K. Siu and J.S. Tse, Ab initio molecular dynamics study on the thermal dissociation of acetic acid 314 (1999) 317
- Liu, Z.F. and S.P. Chan, Dissociative chemisorption of molecular chlorine on Si(100) - a first principles study 318 (2000) 15
- Livshits, A.M. and Yu.E. Lozovik, Coulomb clusters on a sphere: topological classification 314 (1999) 577
- Lledós, A., see Fantacci, S. 315 (1999) 145
- Llopis, J., see García, M.A. 315 (1999) 313
- Li.Tamarit, J., see Céolin, R. 314 (1999) 21
- Löbau, J., see Saß, M. 311 (1999) 13
- Löfken, J.O., see Kolmakov, A. 319 (2000) 465
- Loi, M.A., see Ariu, M. 313 (1999) 405
- Lokhman, V.N., see Dem'yanenko, A.V. 320 (2000) 594
- Lommatzsch, U., E.H. Wahl, T.G. Owano, C.H. Kruger and R.N. Zare, Spatial concentration and temperature distribution of CH radicals formed in a diamond thin-film hot-filament reactor 320 (2000) 339
- Lonfat, M., B. Marsen and K. Sattler, The energy gap of carbon clusters studied by scanning tunneling spectroscopy 313 (1999) 539
- Longo, S., D. Bruno, M. Capitelli and P. Minelli, A Monte Carlo model for the non-equilibrium coherent kinetics of ensembles of two level systems 316 (2000) 311
- Longo, S., see Bruno, D. 320 (2000) 245
- Lopes, M.C.A., see Yench, A.J. 315 (1999) 37
- López, D.O., see Céolin, R. 314 (1999) 21
- López, D.O., see Allouchi, H. 317 (2000) 40
- López, J.C., P.G. Favero, A. Dell'Erba and W. Caminati, An unusual 'ring-puckering': tunneling of Ar in difluoromethane-Ar 316 (2000) 81
- López, M., see Pasqualini, E.E. 320 (2000) 415
- Lou, N.-Q., see Zhu, R. 313 (1999) 98
- Loutts, G.B., see Rakhimov, R.R. 319 (2000) 639
- Lozovik, Yu.E., see Livshits, A.M. 314 (1999) 577
- Lozovsky, V.A., see Derzy, I. 313 (1999) 121
- Lu, H.-F., see Sun, Y.-C. 318 (2000) 7

- Lu, J., X. Zhang and X. Zhao, Electronic structures of endohedral N@C₆₀, O@C₆₀ and F@C₆₀ 312 (1999) 85
- Lu, Q., J. Hu, K. Tang, B. Deng, Y. Qian, G. Zhou and X. Liu, The co-reduction route to TiC nanocrystallites at low temperature 314 (1999) 37
- Lu, W.C., C.C. Sun, Q.J. Zang and C.B. Liu, Theoretical study of the aza-Wittig reaction $X_3P=NH + O=CHCOOH \rightarrow X_3P=O + HN=CHCOOH$ for X = Cl, H and CH₃ 311 (1999) 491
- Lucas, J.M., see Aquilanti, V. 318 (2000) 619
- Lucchese, R.R., see McIntosh, A. 314 (1999) 57
- Lüchow, A., see Sokolova, S. 320 (2000) 421
- Luckhurst, G.R., see Emsley, J.W. 320 (2000) 255
- Luerßen, B., S. Günther, H. Marbach, M. Kiskinova, J. Janek and R. Imbühl, Photoelectron spectroscopy of electrochemically induced oxygen spillover at the Pt/YSZ interface 316 (2000) 331
- Luh, T.-Y., see Hsu, C.-C. 311 (1999) 355
- Lukzen, N.N., see Makarov, T.N. 317 (2000) 252
- Luna, A., M. Alcamí, O. Mó and M. Yáñez, Cu⁺ binding energies. Dramatic failure of the G2 method vs. good performance of the B3LYP approach 320 (2000) 129
- Luo, G.-B., see Wei, T.-X. 319 (2000) 7
- Luo, L., see Li, Q. 320 (2000) 335
- Lutterloh, C., see Dinger, A. 311 (1999) 202
- Lutterloh, C., see Dinger, A. 320 (2000) 405
- Luzzi, D.E., see Smith, B.W. 315 (1999) 31
- L'vov, S.G., see Kukovitsky, E.F. 317 (2000) 65
- Lynden-Bell, R.M., see Alavi, A. 320 (2000) 487
- Lyubovskaya, R.N., see Konarev, D.V. 314 (1999) 570
- Ma, G. and H. Guo, Barrier crossing in a dissipative environment: a reduced density matrix treatment of STM-induced atom transfer dynamics 317 (2000) 315
- Ma, G., see Qian, W. 319 (2000) 89
- Ma, G., see Chen, R. 320 (2000) 567
- Ma, N.L., K.-C. Lau, S.-H. Chien and W.-K. Li, Thermochemistry of hydrochlorofluoromethanes revisited: a theoretical study with the Gaussian-3 (G3) procedure 311 (1999) 275
- Mackay, A.L., see Gandy, P.J.F. 314 (1999) 543
- Mackenzie, J.D., see Silva, C. 319 (2000) 494
- MacNamara, E., C.V. Rice, J. Smith, L.J. Smith and D. Raftery, Cross-relaxation dynamics between laser-polarized xenon and a surface species using a simple three-spin model 317 (2000) 165
- Madden, P.A., see Domene, C. 314 (1999) 158
- Madhu, P.K., see Vinogradov, E. 314 (1999) 443
- Madhu, P.K., see Mandal, P.K. 320 (2000) 269
- Madhu, P.K., see Goldbourt, A. 320 (2000) 448
- Maeda, Y., see Akasaka, T. 319 (2000) 153
- Mafuné, F., see Horimoto, N. 318 (2000) 536
- Mager, O., see Leonhardt, M. 313 (1999) 24
- Magnasco, V. and M. Ottonelli, Dipole polarizability pseudospectra and C₆ dispersion coefficients for two-electron model systems 311 (1999) 407
- Magnier, S., see Kowalczyk, P. 314 (1999) 47
- Mahara, H., T. Yamaguchi and Y. Amagishi, A numerical study of the decomposition of chemical waves in a closed system 317 (2000) 23

- Mahesh, T.S., T.G. Ajithkumar, C.S. Nagaraja, G. Bodenhausen and A. Kumar, Suppression of sidebands in two-dimensional exchange and MQMAS spectroscopies in solids by variable-speed magic-angle sample spinning 319 (2000) 278
- Maheshwari, S., D. Chakraborty and N. Sathyamurthy, Possibility of proton motion through buckminsterfullerene 315 (1999) 181
- Mahrt, R.F., see Wegmann, G. 312 (1999) 376
- Mahrt, R.F., see Harrison, M.G. 313 (1999) 755
- Mahrt, R.F., see Hopmeier, M. 314 (1999) 9
- Maier, J.P., see Pfluger, D. 313 (1999) 171
- Maier, K., see Neeb, M. 320 (2000) 217
- Maigret, B., see Cai, W.-S. 319 (2000) 708
- Maillotte, H., see Chérioux, F. 319 (2000) 669
- Main, J., see Belkić, D. 315 (1999) 135
- Mair, C., see Fiegele, T. 316 (2000) 387
- Majumder, C., S.K. Kulshreshtha, G.P. Das and D.G. Kanhere, Clustering behaviour in bimetallic clusters: a density functional theory based molecular dynamics study 311 (1999) 62
- Makarov, T.N., E.G. Bagryanskaya, S.R. Shakirov, N.N. Lukzen and R.Z. Sagdeev, CIDNP in a double switched magnetic field 317 (2000) 252
- Makoshi, K., see Fukumoto, Y. 313 (1999) 283
- Mallia, G., see Lichanot, A. 318 (2000) 240
- Malrieu, J.-P., see Calzado, C.J. 317 (2000) 404
- Malrieu, J.-P., see Angeli, C. 317 (2000) 472
- Malsch, K., see Krawczyk, R.P. 320 (2000) 535
- Malyshev, V.A. and F. Domínguez-Adame, Motional narrowing effect in one-dimensional Frenkel chains with configurational disorder 313 (1999) 255
- Manaka, T., H. Hoshi, K. Ishikawa, H. Takezoe, S. Koshihara, M. Kira and T. Miyazawa, Large order-disorder transition in polydihexylsilane films as studied by second-harmonic generation spectroscopy 317 (2000) 260
- Manby, F.R. and P.J. Knowles, Erratum to "A real-space perturbation theory for electronic correlation". [Chem. Phys. Lett. 310 (1999) 561-567] 312 (1999) 347
- Mancini, L., see Capuani, S. 316 (2000) 222
- Mandal, A.B., see Geetha, B. 318 (2000) 35
- Mandal, D., see Pal, S.K. 312 (1999) 178
- Mandal, P.K., P.K. Madhu and N. Müller, Nuclear magnetic relaxation of methyl protons in a paramagnetic protein: cross-correlation effects 320 (2000) 269
- Manolopoulos, D.E., see Brinkmann, G. 315 (1999) 335
- Manos, G., see Du, Z. 318 (2000) 319
- Manthe, U., W. Bian and H.-J. Werner, Quantum-mechanical calculation of the thermal rate constant for the $H_2 + Cl \rightarrow H + HCl$ reaction 313 (1999) 647
- Manz, J., see Andrianov, I. 318 (2000) 256
- Mao, B.W., see Cao, P.G. 316 (2000) 1
- Mao, Z., see Sinnott, S.B. 315 (1999) 25
- Mapelli, C., C. Castiglioni and G. Zerbi, Calculation of vibrational cyclic redundancies in planar rings 314 (1999) 189
- Maraviglia, B., see Capuani, S. 316 (2000) 222
- Marbach, H., see Luerßen, B. 316 (2000) 331
- Marchettini, N. and M. Rustici, Effect of medium viscosity in a closed unstirred Belousov-Zhabotinsky system 317 (2000) 649

- Marcus, R.K. and R.W. Schwartz, Compositional profiling of solution-deposited lead zirconate–titanate thin films by radio-frequency glow discharge atomic emission spectroscopy (rf-GD-AES) 318 (2000) 481
- Margrave, J.L., see Kelly, K.F. 313 (1999) 445
- Margulès, L., see Breidung, J. 313 (1999) 713
- Marian, C.M., see Tatchen, J. 313 (1999) 351
- Mark, F., see Kneip, C. 311 (1999) 479
- Märk, T.D., see Fiegele, T. 316 (2000) 387
- Markelz, A.G., A. Roitberg and E.J. Heilweil, Pulsed terahertz spectroscopy of DNA, bovine serum albumin and collagen between 0.1 and 2.0 THz 320 (2000) 42
- Marković, N., see Barinova, Š. 315 (1999) 282
- Maroncelli, M., see Horng, M.L. 315 (1999) 363
- Maroulis, G., Hexadecapole moment, dipole and quadrupole polarizability of sulfur hexafluoride 312 (1999) 255
- Maroulis, G., Is the dipole polarizability of hydrogen iodide accurately known? 318 (2000) 181
- Maroulis, G., see Xenides, D. 319 (2000) 618
- Marowsky, G., see Boneß, J. 313 (1999) 19
- Marsen, B., see Lonfat, M. 313 (1999) 539
- Mårtensson, N., see Föhlisch, A. 315 (1999) 194
- Martin, M.M., see Texier, I. 311 (1999) 139
- Martínez-Haya, B., I. Zapater, P. Quintana, M. Menéndez, E. Verdasco, J. Santamaría, L. Bañares and F.J. Aoiz, Photodissociation of dimethyl sulfide at 227.5 nm: resonance-enhanced multiphoton ionization of the methyl fragment 311 (1999) 159
- Martínez-Núñez, E. and S.A. Vázquez, Rotational effects in the unimolecular dissociation of the acetyl radical 316 (2000) 471
- Martínez Torres, E., Icosahedral hybrid orbitals 320 (2000) 523
- Martins, J.L., see Miao, M.S. 316 (2000) 297
- Martorell, J., see Quitevis, E.L. 319 (2000) 138
- Martynski, T., see Lantz, M.A. 315 (1999) 61
- Marui, S., see Tonokura, K. 313 (1999) 771
- Maruszewski, K., M. Jasiorowski, M. Salamon and W. Stręk, Physicochemical properties of $\text{Ru}(\text{bpy})_3^{2+}$ entrapped in silicate bulks and fiber thin films prepared by the sol–gel method 314 (1999) 83
- Maruyama, Y., see Yamaguchi, W. 311 (1999) 341
- Maruyama, Y., see Yamaguchi, W. 311 (1999) 415
- Maseras, F., see Fantacci, S. 315 (1999) 145
- Maslen, P.E., M.S. Lee and M. Head-Gordon, An accurate local model for triple substitutions in fourth order Møller–Plesset theory and in perturbative corrections to singles and doubles coupled cluster methods 319 (2000) 205
- Masuda, T., see Chin, B.-C. 318 (2000) 499
- Materny, A., see Ermoshin, V.A. 311 (1999) 146
- Materny, A., see Vierheilig, A. 312 (1999) 349
- Mathis, C., see Jouguelet, E. 318 (2000) 561
- Mathur, P., see Philip, R. 313 (1999) 719
- Matsumura, K., see Uchimaru, T. 318 (2000) 203
- Matsumura, K., see Tsuzuki, S. 319 (2000) 547
- Matsuo, A., see Furuya, K. 313 (1999) 559

- Matsushita, Y. and T. Hikida, The effect of cyclodextrin complexation on the fluorescence properties of ethyl-4'-dimethylaminobenzoate 313 (1999) 85
- Mattar, S.M. and A.D. Stephens, UBILYP hybrid density functional studies of the 2,2,6,6-tetramethyl-4-piperidone-oxyl (TEMPONE) hyperfine tensors 319 (2000) 601
- Matusek, D.R., see DiLabio, G.A. 317 (2000) 599
- Mau, A.W.H., see Li, D.-C. 316 (2000) 349
- Maurer, T., see Geiger, H. 314 (1999) 465
- Maurin, G., C. Bousquet, F. Henn, P. Bernier, R. Almairac and B. Simon, Electrochemical intercalation of lithium into multiwall carbon nanotubes 312 (1999) 14
- Maus, M., see Rettig, W. 318 (2000) 173
- Mavrin, B.N., see Chernozatonskii, L.A. 316 (2000) 199
- Mavromanolakis, A., see De Nalda, R. 316 (2000) 449
- Mayama, H., T. Iwataki and K. Yoshikawa, Thermodynamics in the folding phase-transition of single T4DNA molecules in poly(ethylene glycol) solution 318 (2000) 113
- Mayer, D., see Zerulla, D. 311 (1999) 8
- Mayer, P.M., Binding energies of nitrile-containing proton-bound clusters: the performance of HF, MP2 and B3-LYP vs. G2 314 (1999) 311
- Mayer, S.G., C.L. Thomsen, M.P. Philpott and P.J. Reid, The solvent-dependent isomerization dynamics of 4-(dimethylamino)azobenzene (DMAAB) studied by subpicosecond pump-probe spectroscopy 314 (1999) 246
- Mayhew, C.A., see Jarvis, G.K. 320 (2000) 104
- M. Bishop, D. and F.L. Gu, Ab initio and semi-empirical studies of the static polarizability and the second hyperpolarizability of diamond: finite T_d symmetry models from CH_4 to $C_{28}H_{172}$ 317 (2000) 322
- McBranch, D.W., see Wang, H.-L. 315 (1999) 173
- McCaffery, A.J., see Whiteley, T.W.J. 314 (1999) 132
- McCash, E.M., see Eve, J.K. 313 (1999) 575
- McCaw, C.S., see Thorne, J.R.G. 319 (2000) 185
- McCoy, E.F. and M.J. Sykes, The estimation of molecular properties using momentum-space wavefunctions 313 (1999) 707
- McCullen, E.F., see Hsu, C.-L. 316 (2000) 336
- McDowell, C.A., see Ding, S. 320 (2000) 316
- McEwan, M.J., see Milligan, D.B. 319 (2000) 482
- McGarvey, J.J., see Bousseksou, A. 318 (2000) 409
- McGrath, M.P., see Seong, J. 314 (1999) 501
- McHale, J.L., see Streiff, J.H. 312 (1999) 369
- McIntosh, A., T. Walther, R.R. Lucchese, J.W. Bevan, R.D. Suenram and A.C. Legon, The microwave spectrum and ground-state structure of $H_2O \cdots HI$ 314 (1999) 57
- McKee, M.L., see Kwon, O. 313 (1999) 321
- McManus, J., R. Kemp-Harper and S. Wimperis, Second-order quadrupolar-dipolar broadening in two-dimensional multiple-quantum MAS NMR 311 (1999) 292
- McQuarrie, B.R. and P. Brumer, Semiclassical initial value representation techniques for chaotic systems 319 (2000) 27
- McQuillan, A.J., see Degenhardt, J. 311 (1999) 179
- Mebel, A.M., M.Y. Lai and Y.L. Wang, Two-dimensional Ga-induced magic clusters on the Si surface: a density functional study 318 (2000) 27
- Meerts, W.L., see Remmers, K. 317 (2000) 197
- Meghdadi, F., see Ariu, M. 313 (1999) 405

- Mehendale, S.C., see Mishra, S.R. 317 (2000) 510
- Meier, B.H., see Ernst, M. 317 (2000) 583
- Meier, R.J., see Koglin, E. 312 (1999) 284
- Meijer, A.J.H.M., see Farebrother, A.J. 319 (2000) 303
- Meijer, G., see Remmers, K. 317 (2000) 197
- Meijer, G., see van Smaalen, S. 319 (2000) 283
- Meissner, L. and M. Nooijen, The coupled-cluster correction to multi-reference configuration interaction method: application to excited states 316 (2000) 501
- Mejias, J.A., A.J. Berry, K. Refson and D.G. Fraser, The kinetics and mechanism of MgO dissolution 314 (1999) 558
316 (2000) 75
- Melandri, S., see Velino, B.
- Melchior, A., X. Chen, I. Bar and S. Rosenwaks, Alteration of Cl spin-orbit branching ratios via photodissociation of pre-excited fundamental CH_3 stretch of CH_3CFCl_2 315 (1999) 421
- Melo, E., see Osuka, A. 313 (1999) 499
- Melville, T.C. and J.A. Coxon, The first spectroscopic observation of YbS : the $\text{A}0^+ - \text{X}0^+$ visible laser excitation spectrum 318 (2000) 454
- Mendonça, C.R., see Dos Santos Jr., D.S. 317 (2000) 1
- Menéndez, M., see Martínez-Haya, B. 311 (1999) 159
- Menon, M., A.N. Andriotis and G.E. Froudakis, Curvature dependence of the metal catalyst atom interaction with carbon nanotubes walls 320 (2000) 425
- Menzel, D., see Föhlich, A. 315 (1999) 194
- Mérawa, M., see Lichanot, A. 318 (2000) 240
- Merchant, K., see Rector, K.D. 316 (2000) 122
- Merkt, F., see Signorell, R. 312 (1999) 139
- Messina, M., see Adams, J.W. 315 (1999) 266
- Metz, R.B., see Aguirre, F. 318 (2000) 466
- Metzger, R.M., see Kwon, O. 313 (1999) 321
- Meyer, G., see Bartels, L. 313 (1999) 544
- Meyer, H., see Gödicke, B. 318 (2000) 102
- Meyer, H., see Kim, Y. 318 (2000) 522
- Meyer, H., see Fleniken, J. 318 (2000) 529
- Mezei, M., see Jedlovsky, P. 318 (2000) 155
- Miao, M.S., V.E. Van Doren, R. Keuleers, H.O. Desseyn, C. Van Alsenoy and J.L. Martins, Density functional calculations of the structure of crystalline urea under high pressure 316 (2000) 297
- Michael, J.V., S.S. Kumaran, M.-C. Su and K.P. Lim, Thermal rate constants over thirty orders of magnitude for the $\text{I} + \text{H}_2$ reaction 319 (2000) 99
- Mickelson, E.T., see Kelly, K.F. 313 (1999) 445
- Mielewska, B., G.C. King, F.H. Read and M. Zubek, A study of resonance structures in elastic electron scattering by carbon monoxide and molecular nitrogen in the backward direction 311 (1999) 428
- Mielke, Z. and K.G. Tokhadze, Infrared matrix isolation studies of nitrous acid complexes with methane, silane and germane 316 (2000) 108
- Mikalo, R., see Appel, G. 313 (1999) 411
- Mikami, M., see Kawata, M. 313 (1999) 261
- Mikami, M., see Kawata, M. 317 (2000) 515
- Mikami, M., see Tsuzuki, S. 319 (2000) 547
- Milletich, R., see van Smaalen, S. 319 (2000) 283

- Milligan, D.B. and M.J. McEwan, $H_3^+ + O$: an experimental study 319 (2000) 482
- Milman, V., see Winkler, B. 312 (1999) 536
- Milošević, S., see Labazan, I. 320 (2000) 613
- Mimuro, M., see Akimoto, S. 313 (1999) 63
- Mináry, P., see Turi, L. 316 (2000) 465
- Minehardt, T.J. and R.E. Wyatt, Quantum dynamics of intramolecular vibrational energy redistribution for initially excited CC ring modes in 30-mode benzene 312 (1999) 485
- Minelli, P., see Longo, S. 316 (2000) 311
- Mirau, P.A., S.A. Heffner and M. Schilling, Controlling the chain dynamics of polymers at interfaces 313 (1999) 139
- Miret-Artes, S., see Gianturco, F.A. 311 (1999) 255
- Mirkin, N.G., see Qian, W. 315 (1999) 125
- Misaizu, F., see Tsunoyama, H. 316 (2000) 442
- Misawa, K., see Chin, B.-C. 318 (2000) 499
- Mishima, O., see Suzuki, Y. 319 (2000) 81
- Mishra, R.K., Y.-T. Lin and S.-L. Lee, Growth mechanism of C_{28} (Td) fullerene: energetics and transition-state structures analysis 313 (1999) 437
- Mishra, S.R., H.S. Rawat, S.C. Mehendale, K.C. Rustagi, A.K. Sood, R. Bandyopadhyay, A. Govindaraj and C.N.R. Rao, Optical limiting in single-walled carbon nanotube suspensions 317 (2000) 510
- Misoguti, L., see Dos Santos Jr., D.S. 317 (2000) 1
- Mitsui, M., Y. Ohshima, S. Ishiuchi, M. Sakai and M. Fujii, Structural characterization of the acridine- $(H_2O)_n$ ($n = 1-3$) clusters by fluorescence-detected infrared spectroscopy 317 (2000) 211
- Mitsuke, K., see Niikura, H. 317 (2000) 45
- Mittal, J.P., see Gawandi, V.B. 314 (1999) 451
- Mittal, J.P., see Bhasikuttan, A.C. 316 (2000) 67
- Mittal, J.P., see Gawandi, V.B. 318 (2000) 496
- Mittendorfer, F., see Duschek, R. 318 (2000) 43
- Miura, S., see Yoshii, N. 317 (2000) 414
- Miura, Y., S. Kimura, S. Kobayashi, M. Iwamoto, Y. Imanishi and J. Umemura, Negative surface potential produced by self-assembled monolayers of helix peptides oriented vertically to a surface 315 (1999) 1
- Miyake, J., see Lantz, M.A. 315 (1999) 61
- Miyamoto, A., see Shrivastava, K.N. 313 (1999) 279
- Miyauchi, R., see Yoshii, N. 317 (2000) 414
- Miyawaki, J., see Yang, D.-S. 313 (1999) 514
- Miyazaki, T., see Shevtsov, V. 319 (2000) 535
- Miyazawa, T., see Manaka, T. 317 (2000) 260
- Mizutani, M., see Niikura, H. 317 (2000) 45
- Mó, O., see Luna, A. 320 (2000) 129
- Moggio, I., see Lanzani, G. 313 (1999) 525
- Mohallem, J.R., see Gonçalves, C.P. 320 (2000) 118
- Mohamed, M.B., V. Volkov, S. Link and M.A. El-Sayed, The 'lightning' gold nanorods: fluorescence enhancement of over a million compared to the gold metal 317 (2000) 519
- Mohan, H., see Gawandi, V.B. 314 (1999) 451
- Mohan, H., see Gawandi, V.B. 318 (2000) 496
- Mohanty, J.F., Anomalous migration of DNA 316 (2000) 558
- Molina, L.T., see Lee, S.-H. 315 (1999) 7

- Molina, M.J., see Lee, S.-H. 315 (1999) 7
- Moliner, N., see L  tard, J.-F. 313 (1999) 115
- Moliner, V., see Castillo, R. 318 (2000) 270
- M  ller, T., see Kolmakov, A. 319 (2000) 465
- Molski, A., J. Hofkens, T. Gensch, N. Boens and F. De Schryver, Theory of time-resolved single-molecule fluorescence spectroscopy 318 (2000) 325
- Moncorg  , R., see Laroche, M. 311 (1999) 167
- Moncrieff, D., see Cioslowski, J. 316 (2000) 536
- Monobe, T., see Ito, A. 315 (1999) 348
- Mons, M., see Piu  zzi, F. 320 (2000) 282
- Montalenti, F., see Ferrando, R. 315 (1999) 153
- Montgomery Jr., H.E., One-electron wavefunctions: variational perturbation theory 311 (1999) 367
- Monthieux, M., see Smith, B.W. 315 (1999) 31
- Moore, E.A., Absolute ^{15}N shielding in dinitrogen trioxide: recalculation of the shielding tensors 317 (2000) 360
- Moos, G., see Hertel, T. 320 (2000) 359
- Morawski, O., see Prochorow, J. 316 (2000) 24
- Mordzinski, A., see Nosenko, Y. 315 (1999) 87
- Moriarty, N.W., see Krokidis, X. 314 (1999) 534
- Morita, T., see Nishikawa, K. 316 (2000) 238
- Morokuma, K., see Karadakov, P.B. 317 (2000) 591
- Morrison, I., see Jenkins, S. 317 (2000) 97
- Morse, M.D., see Fabbi, J.C. 320 (2000) 303
- Moscard  , F., see Sancho-Garc  a, J.C. 317 (2000) 245
- Moses, D., A. Dogariu and A.J. Heeger, Ultrafast photoinduced charge generation in conjugated polymers 316 (2000) 356
- Moss, R.E., On the fully nonadiabatic dipole polarizability of $\text{H}_2^+(0,0)$ 311 (1999) 231
- Moss, R.E., see Bunker, P.R. 316 (2000) 266
- Moszynski, R., see Rode, M. 314 (1999) 326
- Mota, F., see Novoa, J.J. 318 (2000) 345
- Moulton, V., see Koolen, J.H. 320 (2000) 213
- Moussa, F., see C  olin, R. 314 (1999) 21
- Moustafa, H., see Abu-Eittah, R.H. 318 (2000) 276
- Msezane, A.Z., see Vranceanu, D. 311 (1999) 395
- Mukai, K., M. Yanagimoto, Y. Shimobe, K. Inoue and Y. Hosokoshi, Doping effect of magnetic impurities on the spin-Peierls compound *p*-CyDOV 311 (1999) 446
- Mukai, K., see Ohara, K. 317 (2000) 621
- Mukamel, S., see Chernyak, V. 319 (2000) 261
- Mukherjee, D., see Kutzelnigg, W. 317 (2000) 569
- Mukherjee, R.K., see Jana, S. 320 (2000) 289
- Mukherjee, T., see Gangopadhyay, D. 318 (2000) 161
- M  llen, K., see Wegmann, G. 312 (1999) 376
- M  llen, K., see Silva, C. 319 (2000) 494
- M  ller, B.R., G. Leibeling and E.-G. J  ger, Cooperative magnetic behavior of self-assembled iron(II) chelate chain compounds 319 (2000) 368
- M  ller-Dethlefs, K., see Dessent, C.E.H. 315 (1999) 103
- M  ller-Dethlefs, K., see Dessent, C.E.H. 319 (2000) 375
- M  ller, H.S.P., Infrared spectroscopy and molecular properties of chlorosyl fluoride, FCIO 314 (1999) 396

- Müller, M., H.-J. Bär, S.M. Kast and J. Brickmann, Ab initio localisation of adsorption sites in guest/host systems: application to the system thionine in zeolite NaY 311 (1999) 485
- Müller, N., see Mandal, P.K. 320 (2000) 269
- Müllerová, A., see Juha, L. 313 (1999) 431
- Mungle, C., see Grimes, C.A. 319 (2000) 460
- Münster, A.F., Comment on "On the nature of patterns arising during polymerization of acrylamide in the presence of the methylene blue–sulfide–oxygen oscillating reaction". [Chem. Phys. Lett. 295 (1998) 70–74] 311 (1999) 102
- Münster, A.F., see Guderian, A. 312 (1999) 440
- Münster, A.F., see Fecher, F. 313 (1999) 205
- Mura, A., see Ariu, M. 313 (1999) 405
- Murad, S. and S. Gupta, A simple molecular dynamics simulation for calculating Henry's constant and solubility of gases in liquids 319 (2000) 60
- Murakami, J., see Yamaguchi, W. 311 (1999) 341
- Murakami, J., see Yamaguchi, W. 311 (1999) 415
- Muraoka, K., see Furukawa, K. 318 (2000) 22
- Murasaki, T., see Tonokura, K. 319 (2000) 507
- Musiał, M., S.A. Kucharski and R.J. Bartlett, T_5 operator in coupled cluster calculations 320 (2000) 542
- Musso, G.F., see Lanzani, G. 313 (1999) 525
- Muthu, D.V.S., see Teredesai, P.V. 319 (2000) 296
- Myers, D.J., M. Shigeiwa, M.D. Fayer and R. Silbey, Non-exponential relaxation of a single quantum vibrational excitation of a large molecule in collision free gas phase at elevated temperature 312 (1999) 399
- Myers, D.J., M. Shigeiwa, M.D. Fayer and B.J. Cherayil, Density dependent vibrational relaxation in supercritical fluids 313 (1999) 592
- Myszkiewicz, G. and J. Sadlej, Ab initio study for the intermolecular potential of the water–nitric oxide complex 318 (2000) 232
- Nabighian, E. and X.D. Zhu, Diffusion of Xe on Ni(111) 316 (2000) 177
- Nachtigall, P., see Bludský, O. 318 (2000) 607
- Nag, K., see Ostrovsky, S.M. 320 (2000) 295
- Nagae, H., see Onaka, K. 315 (1999) 75
- Nagao, H., see Shigeta, Y. 315 (1999) 441
- Nagao, H., see Soda, T. 319 (2000) 223
- Nagaraja, C.S., see Mahesh, T.S. 319 (2000) 278
- Nagarajan, V., System–bath coupling dynamics by femtosecond pump–probe spectroscopy 317 (2000) 203
- Nagaraju, N., see Willems, I. 317 (2000) 71
- Nagasawa, Y., Y. Ando and T. Okada, Solvent dependence of ultrafast ground state recovery of the triphenylmethane dyes, brilliant green and malachite green 312 (1999) 161
- Nagasawa, Y., see Yamaguchi, Y. 316 (2000) 477
- Nagase, S., see Kobayashi, K. 313 (1999) 45
- Nagase, S., see Akasaka, T. 319 (2000) 153
- Nagesha, K. and L.A. Pinnaduwege, Magnetic and electric field-induced enhancements in laser-induced anion formation 312 (1999) 19
- Naik, D.B. and W. Schnabel, Photoionization of $\text{Ru}(\text{bpy})_3^{2+}$ ions in aqueous solutions containing sodium dodecyl sulfate. Influence of ion binding 315 (1999) 416
- Naik, P.D., see Dhanya, S. 318 (2000) 125
- Naito, M., H. Okamoto and N. Tanaka, Nonlinear dynamical analysis of spike generation in electrochemical oxidation of formic acid on Pt 319 (2000) 71

- Nakagaki, R., see Kohtani, S. 316 (2000) 88
- Nakahara, H., see Akiyama, K. 317 (2000) 490
- Nakahara, H., see Kikuchi, K. 319 (2000) 472
- Nakai, H. and Y. Kawamura, π - σ Hyperconjugation mechanism on the rotational barrier of the methyl group (II): 1- and 2-methylnaphthalenes in the S_0 , S_1 , C_0 , and A_1 states 318 (2000) 298
- Nakai, T., see Nakazawa, Y. 311 (1999) 362
- Nakajima, N., see Ono, S. 312 (1999) 247
- Nakamura, C., see Lantz, M.A. 315 (1999) 61
- Nakamura, H., see Ono, S. 312 (1999) 247
- Nakano, M., M.-B. Song and M. Ito, Hydrogen bonding between a water molecule and electronegative additives (O or Cl⁻) on a Pt(111) surface 320 (2000) 381
- Nakanaga, T., see Ito, F. 318 (2000) 571
- Nakano, H. and K. Hirao, A quasi-complete active space self-consistent field method 317 (2000) 90
- Nakano, M., S. Yamada and K. Yamaguchi, Theoretical studies on second hyperpolarizabilities for cation radical states of tetrathiafulvalene and tetrathiapentalene 311 (1999) 221
- Nakano, M. and K. Yamaguchi, Electron-correlation dynamics of a one-dimensional H_2 model in a quantized photon field 317 (2000) 103
- Nakano, T., T. Kaminuma, T. Sato, Y. Akiyama, M. Uebayasi and K. Kitaura, Fragment molecular orbital method: application to polypeptides 318 (2000) 614
- Nakano, T., see Kitaura, K. 312 (1999) 319
- Nakano, T., see Kitaura, K. 313 (1999) 701
- Nakao, K., see Kurita, N. 313 (1999) 693
- Nakashima, N., see Shimizu, S. 317 (2000) 611
- Nakatsuji, H., see Hu, Z.-M. 313 (1999) 14
- Nakatsuka, H., see Ye, J.Y. 320 (2000) 607
- Nakayama, H., K. Saitow, M. Sakashita, K. Ishii and K. Nishikawa, Raman spectral changes of neat CO_2 across the ridge of density fluctuation in supercritical region 320 (2000) 323
- Nakazaki, J., Y. Ishikawa, A. Izuoka, T. Sugawara and Y. Kawada, Preparation of isolable ion-radical salt derived from TTF-based spin-polarized donor 319 (2000) 385
- Nakazawa, Y., T. Nakai, T. Kameda and T. Asakura, A ^{13}C NMR study on the structural change of silk fibroin from *Samia cynthia ricini* 311 (1999) 362
- Nam, K.-Y., J.H. Yoon and K.T. No, Intra ion-ion interactions in aqueous solution: β -alanine zwitterion and 1,2-ethenediammonium 319 (2000) 391
- Naqvi, K.R., see Osuka, A. 313 (1999) 499
- Narayan, K.S., see Vijaya Sarathy, K. 318 (2000) 543
- Nath, M., see Govindaraj, A. 317 (2000) 35
- Nee, J.B., C.T. Kuo, H.C. Tseng and S.Y. Wang, Potential energy curves of Xe_2 derived from the pressure-dependent fluorescence excitation spectra of the 1st and 2nd continuum 318 (2000) 402
- Neeb, M., A. Kivimäki, B. Kempgens, H.M. Köppe, K. Maier, A.M. Bradshaw and N. Kosugi, Partial electron yield spectrum of N_2 : doubly excited states at the K-shell threshold 320 (2000) 217
- Németh, K., see Kneip, C. 311 (1999) 479
- Nest, M., U. Kleinekathöfer, M. Schreiber and P. Saalfrank, The mapped Fourier method for scattering problems 313 (1999) 665
- Netzer, F.P., see Duschek, R. 318 (2000) 43
- Neukermans, S., see Bouwen, W. 314 (1999) 227
- Neumann, M.A., see Plazanet, M. 320 (2000) 651

- Neuwahl, F.V.R., P. Foggi and R.G. Brown, Sub-picosecond and picosecond dynamics in the S_1 state of [2,2'-bipyridyl]-3,3'-diol investigated by UV-visible transient absorption spectroscopy 319 (2000) 157
- Newell, W.R., see El-Zein, A. 319 (2000) 701
- Neyer, D.W., see Teule, J.M. 320 (2000) 177
- Ng, C.-Y., see Peterka, D.S. 312 (1999) 108
- Ng, C.Y., see Shiell, R.C. 315 (1999) 390
- Nguyen, M.T. and T.-K. Ha, Theoretical study of the pentanitrogen cation (N_5^+) 317 (2000) 135
- Nguyen, M.T., see Ha, T.-K. 315 (1999) 327
- Nibbering, E., see Fiedor, L. 319 (2000) 145
- Nibbering, E.T.J., see Tschirschwitz, F. 312 (1999) 169
- Nibbering, N.M.M., see Sarobe, M. 313 (1999) 31
- Nie, X., see Heinze, S. 315 (1999) 167
- Niedner-Schatteburg, G., see Achatz, U. 320 (2000) 53
- Nielsen, N.C., see Rasmussen, J.T. 314 (1999) 239
- Nielsen, O.J., see Wallington, T.J. 313 (1999) 456
- Nielsen, S.B., see Ayotte, P. 316 (2000) 455
- Niikura, H., M. Mizutani and K. Mitsuke, Rotational state distribution of N_2^+ produced from N_2 or N_2O observed by a laser-synchrotron radiation combination technique 317 (2000) 45
- Nikitin, E.E., see Ohmori, K. 315 (1999) 411
- Nikl, M., see Babin, V. 314 (1999) 31
- Nikolaev, P., M.J. Bronikowski, R.K. Bradley, F. Rohmund, D.T. Colbert, K.A. Smith and R.E. Smalley, Gas-phase catalytic growth of single-walled carbon nanotubes from carbon monoxide 313 (1999) 91
- Nikolaev, P., see Iliev, M.N. 316 (2000) 217
- Nikolaev, P., see Arepalli, S. 320 (2000) 26
- Nikoobakht, B., see Link, S. 315 (1999) 12
- Nilsson, A., see Föhlich, A. 315 (1999) 194
- Nilsson, L., see Lahiri, A. 311 (1999) 459
- Ning, C.G., see Deng, J.K. 313 (1999) 134
- Nishijo, J., see Hasegawa, T. 317 (2000) 644
- Nishikawa, H., see Kikuchi, K. 319 (2000) 472
- Nishikawa, K. and T. Morita, Inhomogeneity of molecular distribution in supercritical fluids 316 (2000) 238
- Nishikawa, K., see Ohta, Y. 316 (2000) 551
- Nishikawa, K., see Nakayama, H. 320 (2000) 323
- No, K.T., see Nam, K.-Y. 319 (2000) 391
- Noid, D.W., K. Fukui, B.G. Sumpter, C. Yang and R.E. Tuzun, Time-averaged normal coordinate analysis of polymer particles and crystals 316 (2000) 285
- Noid, D.W., see Ford, J.V. 316 (2000) 181
- Nonose, S., see Ingólfsson, O. 311 (1999) 421
- Nooijen, M., see Meissner, L. 316 (2000) 501
- Nosenko, Y., Y. Stepanenko, F. Wu, R.P. Thummel and A. Mordzinski, Laser studies of pyridylindoles in supersonic jets 315 (1999) 87
- Noto, R., see Cottone, G. 319 (2000) 51
- Novaro, O., see Bravo-Pérez, G. 313 (1999) 655
- Novoa, J.J. and F. Mota, The C-H... π bonds: strength, identification, and hydrogen-bonded nature: a theoretical study 318 (2000) 345

- Nowak, C., see Kolmakov, A. 319 (2000) 465
Nowak, W., see Szubiakowski, J. 313 (1999) 473
Nozaki, K., see Shiratori, H. 320 (2000) 631
Nyman, G., see Yu, H.-G. 312 (1999) 585
Nyman, G., see Barinovsky, G. 315 (1999) 282
- Obi, K., see Kawai, A. 318 (2000) 85
- Ochimizu, T., K. Seki, M. Yagi, J.B. Halpern and H. Okabe, Rate constants for the reactions of CN with C_6-C_8 unsaturated hydrocarbons: the relations between the reaction rates and the molecular lengths 313 (1999) 451
- Oestreich, M., see Wegmann, G. 312 (1999) 376
- Oestreich, M., see Hopmeier, M. 314 (1999) 9
- Ogawa, T., see Furuya, K. 313 (1999) 559
- Ogawa, T., see Zheng, X.-Y. 316 (2000) 6
- Ogawa, T., see Furuya, K. 319 (2000) 335
- Ogura, S., see Kohno, M. 319 (2000) 451
- Ogurok, D.D., see Dem'yanenko, A.V. 320 (2000) 594
- Ohara, K. and K. Mukai, Anomalous spin polarization in the photoreduction of chromone-2-carboxylic acid with alcohol induced by hydrochloric acid 317 (2000) 621
- Ohkoshi, S. and K. Hashimoto, Ferromagnetism of cobalt-chromium polycyanides 314 (1999) 210
- Ohkubo, T., T. Iiyama and K. Kaneko, Organized structures of methanol in carbon nanospaces at 303 K studies with in situ X-ray diffraction 312 (1999) 191
- Ohmori, K., T. Kurosawa, H. Chiba, M. Okunishi, Y. Sato, A.Z. Devdariani and E.E. Nikitin, Far-wing excitation study on the transition regions of the metastable mercury atom collisions: $Hg(6^3P_2) + N_2$ and CO 315 (1999) 411
- Ohno, K., see Tsunoyama, H. 316 (2000) 442
- Ohno, T., see Shiratori, H. 320 (2000) 631
- Ohoyama, H., H. Kawaguchi, M. Yamato, T. Kasai, B.G. Brunetti and F. Vecchiocattivi, Evidence for steric effect in methyl chloride ionization by metastable argon atoms 313 (1999) 484
- Ohshima, K., see Ikeda, T. 318 (2000) 93
- Ohshima, Y., see Kawashima, Y. 315 (1999) 201
- Ohshima, Y., see Mitsui, M. 317 (2000) 211
- Ohshimo, K., see Tsunoyama, H. 316 (2000) 442
- Ohta, N., H. Kawabata, S. Umeuchi and I. Yamazaki, Erratum to: "Efficient fatigue of excimer fluorescence by an electric field and generation of electroluminescence of 1,3-bis-(1-pyrenyl)propane in a PMMA polymer film". [Chem. Phys. Lett. 310 (1999) 397-404] 315 (1999) 151
- Ohta, Y., T. Yoshimoto and K. Nishikawa, One approach to the control of intramolecular hydrogen transfer 316 (2000) 551
- Ohtake, T., N. Sonoyama and T. Sakata, Electrochemical luminescence of $ZnGa_2O_4$ semiconductor electrodes activated with Cr and Co 318 (2000) 517
- Oka, H., see Amano, T. 311 (1999) 433
- Okabe, H., see Ochimizu, T. 313 (1999) 451
- Okada, M., see Saito, K. 318 (2000) 75
- Okada, T., see Nagasawa, Y. 312 (1999) 161
- Okamoto, H., see Naito, M. 319 (2000) 71
- Okamoto, Y., see Sugita, Y. 314 (1999) 141
- Okazaki, S., see Yoshii, N. 317 (2000) 414

- Okazaki, T., Y. Lian, Z. Gu, K. Suenaga and Hisanori Shinohara, Isolation and spectroscopic characterization of Sm-containing metallofullerenes 320 (2000) 435
- Oki, N., see Kawai, A. 318 (2000) 85
- Okubo, S., see Akasaka, T. 319 (2000) 153
- Okumura, K., A. Tokmakoff and Y. Tanimura, Two-dimensional line-shape analysis of photon-echo signal 314 (1999) 488
- Okunishi, M., see Ohmori, K. 315 (1999) 411
- Oleinikova, A. and H. Weingärtner, Isotope effect on the coexistence curve and crossover behavior of water + tetrahydrofuran 319 (2000) 119
- Oliva, M., see Safont, V.S. 318 (2000) 361
- Oliveira Jr., O.N., see Leite, V.B.P. 316 (2000) 343
- Oliveira Jr., O.N., see Dos Santos Jr., D.S. 317 (2000) 1
- Olkhov, R.V. and O. Dopfer, Spectroscopic and ab initio studies of ionic hydrogen bonds: the O–H stretch vibration of $\text{SiOH}^+ - \text{X}$ dimers ($\text{X} = \text{He}, \text{Ne}, \text{Ar}, \text{N}_2$) 314 (1999) 215
- Olsen, J., see Bak, K.L. 317 (2000) 116
- Olsen, J., see Halkier, A. 319 (2000) 287
- Olsen, J., see Bak, K.L. 319 (2000) 563
- Olsson, E., see Liu, B. 320 (2000) 365
- Onaka, K., R. Fujii, H. Nagae, M. Kuki, Y. Koyama and Y. Watanabe, The state energy and the displacements of the potential minima of the 2A_g^- state in all-*trans*- β -carotene as determined by fluorescence spectroscopy 315 (1999) 75
- Ong, P.P., see Tan, T.L. 315 (1999) 82
- Onishi, T., see Soda, T. 319 (2000) 223
- Ono, S., N. Nakajima, J. Higo and H. Nakamura, The multicanonical weighted histogram analysis method for the free-energy landscape along structural transition paths 312 (1999) 247
- Onoe, J., Y.-i. Hashi, K. Esfarjani, T. Hara, Y. Kawazoe and K. Takeuchi, In-situ infrared spectroscopy of a photoirradiated potassium-doped C_{60} film 315 (1999) 19
- Oppel, M. and G.K. Paramonov, Selective vibronic excitation and bond breaking by picosecond UV and IR laser pulses: application to a two-dimensional model of HONO_2 313 (1999) 332
- Orbán, M., see Kurin-Csörgei, K. 311 (1999) 105
- Oref, I., see Bernshtein, V. 313 (1999) 52
- Orlando, J.J., see Burkholder, J.B. 317 (2000) 605
- Orlando, R., see Lichanot, A. 318 (2000) 240
- Ornellas, F.R., see Resende, S.M. 318 (2000) 340
- Orr, B.J., see He, Y. 319 (2000) 131
- Orr-Ewing, A.J., see Regan, P.M. 315 (1999) 187
- Ortiz-López, J., see Venegas, V. 318 (2000) 655
- Osmann, G., P.R. Bunker, W.P. Kraemer and P. Jensen, Coulomb explosion imaging: the CH_2^+ , H_2O^+ and NH_2^+ ions as benchmarks 318 (2000) 597
- Ostrovsky, S.M., R. Werner, K. Nag and W. Haase, Electron localization–delocalization in mixed-valence iron dimers 320 (2000) 295
- Osuka, A., T. Kume, G.W. Haggquist, T. Javorfi, J.C. Lima, E. Melo and K.R. Naqvi, Photophysical characteristics of two model antenna systems: a fucoxanthin–pyropheoporbide dyad and its peridinin analogue 313 (1999) 499
- Osuka, A., see Shiratori, H. 320 (2000) 631
- Oswald, R., see Botschwina, P. 319 (2000) 587
- Ottinger, C., M. Brozis and A. Kowalski, Hot-atom chemiluminescence: a beam study of the reaction $\text{N}(^4\text{S}) + \text{H}_2 \rightarrow \text{NH}(\text{A}^3\Pi) + \text{H}$ 315 (1999) 355

- Ottinger, Ch. and T. Winkler, The vibrational level structure of *trans*-glyoxal in the T_1 (3A_u) state 314 (1999) 411
- Otto, P., see Hu, A. 320 (2000) 6
- Ottolenghi, M., see Ye, T. 314 (1999) 429
- Ottonelli, M., see Magnasco, V. 311 (1999) 407
- Ouyang, G., see Chen, X.J. 319 (2000) 76
- Owano, T.G., see Zhao, M. 318 (2000) 555
- Owano, T.G., see Lommatzsch, U. 320 (2000) 339
- Ozaki, A., see Shrivastava, K.N. 313 (1999) 279
- Paa, W., see Yang, J.-P. 320 (2000) 665
- Pacchioni, G., see Soave, R. 320 (2000) 345
- Paci, M., see Capuani, S. 316 (2000) 222
- Paesani, F., see Gianturco, F.A. 311 (1999) 255
- Painelli, A. and F. Terenziani, A non-perturbative approach to solvatochromic shifts of push-pull chromophores 312 (1999) 211
- Painter, A.J., see Duer, M.J. 313 (1999) 763
- Paje, S.E., see García, M.A. 315 (1999) 313
- Pal, S.K., D. Mandal, D. Sukul and K. Bhattacharyya, Solvation dynamics of 4-(dicyanomethylene)-2-methyl-6-(*p*-dimethylaminostyryl)-4H-pyran (DCM) in a microemulsion 312 (1999) 178
- Palit, D.K., see Bhasikuttan, A.C. 316 (2000) 67
- Palmer, P.M., Y. Chen and M.R. Topp, Simple water clusters of Coumarins 151 and 152A studied by IR-UV double resonance spectroscopy 318 (2000) 440
- Palmer, R.E., see Robinson, A.P.G. 312 (1999) 469
- Palmieri, P., see Aquilanti, V. 318 (2000) 619
- Palser, A.H.R., see Brinkmann, G. 315 (1999) 335
- Paluch, M., see Corezzi, S. 320 (2000) 113
- Pan, D., L.C.T. Shoute and D.L. Phillips, Time-resolved resonance Raman and density functional study of the radical cations of chlorobiphenyls 316 (2000) 395
- Pan, D. and D.L. Phillips, Investigation of the effects of substitution position on the radical anions of chlorobiphenyls 318 (2000) 214
- Pan, J.-F., S.-J. Chua and W. Huang, Conformational analysis of trimethylsilyl-substituted *trans*-stilbenes: modeling of torsions in silicon-containing poly(*para*-phenylenevinylene) 315 (1999) 233
- Pan, Z.-X., see Cai, W.-S. 319 (2000) 708
- Panten, D., G. Chambaud, P. Rosmus and P.J. Knowles, Rovibronic states of the $X^2\Pi$ state of CCO^- 311 (1999) 390
- Papadopoulos, M.G., see Inlgamells, V.E. 316 (2000) 541
- Paramonov, G.K., see Oppel, M. 313 (1999) 332
- Parilla, P.A., see Dillon, A.C. 316 (2000) 13
- Park, G.-S., see Lee, C.J. 312 (1999) 461
- Park, J.K., Potential energy curves for the dissociation of the Rydberg H_3O radical into ($H_2O + H$) 315 (1999) 119
- Park, Y.S., see Lee, C.J. 312 (1999) 461
- Parson, R., see Sanov, A. 313 (1999) 812
- Parsons, B., L.J. Butler, D. Xie and H. Guo, A combined experimental and theoretical study of resonance emission spectra of $SO_2(\tilde{C}^1B_2)$ 320 (2000) 499
- Pascoli, G. and H. Lavendy, Are C_nN^- clusters really bent? 312 (1999) 333

- Pashov, A., see Kowalczyk, P. 314 (1999) 47
- Pasqualini, E.E. and M. López, Neutral carbon chain free energies 320 (2000) 415
- Pastorino, C. and Z. Gamba, Test of a simple and flexible S_8 model molecule in α - S_8 crystals 319 (2000) 20
- Patton, K., see Kim, Y. 318 (2000) 522
- Patwari, G.N., S. Doraiswamy and S. Wategaonkar, IVR in the S_1 state of jet-cooled *cis*- and *trans*-*p*-dimethoxybenzene 316 (2000) 433
- Paul, H., see Savitsky, A.N. 319 (2000) 403
- Pavel, M., see Juha, L. 313 (1999) 431
- Pazzi, G.P., see Babin, V. 314 (1999) 31
- Péchy, P., see Donzé, N. 315 (1999) 405
- Peck, J.R., X.L. Peng, L.W. Anderson and J.E. Lawler, Ultraviolet reflection–absorption spectroscopy of C_6H_6 physisorbed on gold 318 (2000) 476
- Pedrielli, P., see Emsley, J.W. 320 (2000) 255
- Peebles, S.A. and R.L. Kuczkowski, Rotational spectrum, structure and modeling of an isomer of the HCCH–OCS dimer 312 (1999) 357
- Pelmenschikov, A., I. Zilberberg, J. Leszczynski, A. Famulari, M. Sironi and M. Raimondi, *cis*-[Pt(NH₃)₂]²⁺ coordination to the N7 and O6 sites of a guanine–cytosine pair: disruption of the Watson–Crick H-bonding pattern 314 (1999) 496
- Peluso, A., see Rassat, A. 313 (1999) 582
- Peng, B., see Dai, Z. 317 (2000) 9
- Peng, H.Y., see Tang, Y.H. 314 (1999) 16
- Peng, H.Y., see Zhou, X.T. 318 (2000) 58
- Peng, L.L., see Chen, X.J. 319 (2000) 76
- Peng, X., see Castle, K.J. 318 (2000) 565
- Peng, X.L., see Peck, J.R. 318 (2000) 476
- Perera, S.A. and R.J. Bartlett, Coupled-cluster calculations of Raman intensities and their application to N_4 and N_5^- 314 (1999) 381
- Pérez-Jiménez, A.J., see Sancho-García, J.C. 317 (2000) 245
- Pérez-Jiménez, A.J., see Sancho-García, J.C. 318 (2000) 649
- Pérez, J.J., see Corcho, F.J. 319 (2000) 65
- Perkins, J.D., see Dillon, A.C. 316 (2000) 13
- Perkins, T.L., see Verdal, N. 320 (2000) 95
- Pernpointner, M. and P. Schwerdtfeger, Extension of the PCNQM model for the calculation of electric field gradient tensors in asymmetric molecules. The carbon electric field gradient in CH₃CHFCI 316 (2000) 141
- Peroncelli, L., see Grossi, G. 313 (1999) 639
- Peterka, D.S., M. Ahmed, C.-Y. Ng and A.G. Suits, Dissociative photoionization dynamics of SF₆ by ion imaging with synchrotron undulator radiation 312 (1999) 108
- Peterka, D.S., see Ahmed, M. 317 (2000) 264
- Peterson, K.A., see Skokov, S. 312 (1999) 494
- Petit, J.-C., see Angeli, F. 320 (2000) 681
- Petit, P., see Jouguelet, E. 318 (2000) 561
- Péto, M., see Berthault, P. 314 (1999) 52
- Pettersson, J.B.C., see Bolton, K. 312 (1999) 71
- Pettersson, L.G.M., T. Hatsui and N. Kosugi, Ni 2p–3d photoabsorption and strong charge transfer satellites in divalent Ni complexes with molecular ligands. Evaluation of π -back donation based on the density functional theory approach 311 (1999) 299

- Pettersson, M., see Isoniemi, E. 311 (1999) 47
- Pettersson, M., see Khriachtchev, L. 316 (2000) 115
- Pevenage, D., M. Van der Auweraer and F.C. De Schryver, Intramolecular photo-induced electron transfer between pyrene and a xanthene dye 319 (2000) 512
- Peverall, R., see Barry, H.R. 319 (2000) 125
- Peyerimhoff, S.D., see Filatov, M. 316 (2000) 135
- Peyghambarian, N., see Golemme, A. 319 (2000) 655
- Pfeiffer, M., see Hogiu, S. 312 (1999) 407
- Pfluger, D., W.E. Sinclair, H. Linnartz and J.P. Maier, Rotationally resolved electronic absorption spectra of triacetylene cation in a supersonic jet 313 (1999) 171
- Pham, T.-A., T. Barisien, V. Grayer, L. Guidoni, G. Hadzioannou and J.-Y. Bigot, Gain dynamics in oriented thin films of an oligo(*para*-phenylene vinylene) 318 (2000) 459
- Philip, R., G. Ravindra Kumar, P. Mathur and S. Ghosh, Non-linear optical properties of the mixed-metal mixed-chalcogen clusters $[\text{Fe}_2(\text{CO})_6\{\mu\text{-SeC}(\text{Ph})=\text{C}(\text{Se})\}(\text{OEt})\text{C}=\text{Cr}(\text{CO})_5]$ and $[\text{Fe}_2(\text{CO})_6\text{Se}_2\{\mu\text{-(CO)}_3\text{Cr}(\eta^5\text{-C}_5\text{H}(\text{CH}_2\text{Ph})(\text{Ph})(\text{OEt}))\}]$ 313 (1999) 719
- Phillips, D.L., see Zheng, X. 313 (1999) 467
- Phillips, D.L., see Pan, D. 316 (2000) 395
- Phillips, D.L., see Zheng, X. 316 (2000) 524
- Phillips, D.L., see Pan, D. 318 (2000) 214
- Phillips, L.F., Capillary waves, slope correlations, and evaporation at the surface of a drop 320 (2000) 398
- Philp, D., see Robinson, A.P.G. 312 (1999) 469
- Philpott, M.P., see Mayer, S.G. 314 (1999) 246
- Piaggi, A., see Ariu, M. 313 (1999) 405
- Piccirillo, S., see Satta, M. 316 (2000) 94
- Pichler, G., see Ban, T. 313 (1999) 110
- Pickard, C.J., see Winkler, B. 312 (1999) 536
- Picucci, F., see Kolmakov, A. 319 (2000) 465
- Piest, H., see Remmers, K. 317 (2000) 197
- Pines, A., see Bush, S.D. 311 (1999) 379
- Pinnaduwa, L.A., see Nagesha, K. 312 (1999) 19
- Pisano, P.J., M.S. Westley and P.L. Houston, The NO vibrational state distribution in the reaction $\text{O}(^1\text{D}) + \text{N}_2\text{O} \rightarrow 2\text{NO}$ 318 (2000) 385
- Piszczek, G., see Kuśba, J. 319 (2000) 661
- Pittner, J., see Andrianov, I. 318 (2000) 256
- Piuzzi, F., I. Dimicoli, M. Mons, B. Tardivel and Q. Zhao, A simple laser vaporization source for thermally fragile molecules coupled to a supersonic expansion: application to the spectroscopy of tryptophan 320 (2000) 282
- Pizzoferrato, R., see Casalboni, M. 319 (2000) 107
- Plaza, P., see Texier, I. 311 (1999) 139
- Plazanet, M., M.A. Neumann and H.P. Trommsdorff, Methyl group rotational tunneling in vibrational spectra of crystals at low temperatures 320 (2000) 651
- Pliego Jr., J.R., Electronic spectra of the $\text{CH}_3\text{C}=\text{N}=\text{CXY}$ ($\text{X}, \text{Y} = \text{H}, \text{Cl}$) nitrile ylides: an ab initio multiconfigurational second-order quasidenerate perturbation theory study 318 (2000) 142
- Pokorná, Z., see Juha, L. 313 (1999) 431
- Polavarapu, P.L., D.K. Chakraborty and K. Ruud, Molecular optical rotation: an evaluation of semiempirical models 319 (2000) 595
- Polyansky, O.L., see Császár, A.G. 312 (1999) 613
- Polyansky, O.L., see Kain, J.S. 317 (2000) 365

- Poovey Jr., R.A., see Adams, J.W. 315 (1999) 266
- Pople, J.A., see Curtiss, L.A. 313 (1999) 600
- Pople, J.A., see Curtiss, L.A. 314 (1999) 101
- Port, H., see Leonhardt, M. 313 (1999) 24
- Port, H., see Seibold, M. 314 (1999) 65
- Portella-Oberli, M.T., see Jeannin, C. 316 (2000) 51
- Potrzebowski, M.J., C. Schneider and P. Tekely, Hydrogen bonding pattern in *N*-benzoyl-(-DL)-L-phenylalanines as revealed by solid-state NMR spectroscopy 313 (1999) 569
- Pradeep, T., see Selvan, R. 316 (2000) 205
- Pradère, F., see Vach, H. 314 (1999) 552
- Pranszke, B., P. Kierzkowski and A. Kowalski, Electronic branching ratios in chemiluminescence from the collisions of $\text{Ca}^*(^3\text{P}_J, ^1\text{D}_2)$ atoms with halogenated methanes $\text{CX}_{4-n}\text{Y}_n$ (X, Y = F, Cl, Br) 317 (2000) 220
- Pratt, D.A., see DiLabio, G.A. 311 (1999) 215
- Pratt, S.T., see Bacon, J.A. 311 (1999) 346
- Preece, J.A., see Robinson, A.P.G. 312 (1999) 469
- Price, S.D., see Kaltsoyannis, N. 313 (1999) 679
- Prochorow, J., I. Deperasińska and O. Morawski, Fluorescence excitation and fluorescence spectra of jet-cooled acridine molecules: acridine dimer formation and structure 316 (2000) 24
- Proos, R.J., see Fono, L. 311 (1999) 131
- Prosmiiti, R., S.C. Farantos and H. Guo, Assigning the transition from normal to local vibrational mode in SO_2 by periodic orbits 311 (1999) 241
- Pusiol, D.J. and F. Vaca Chávez, NMR study of the director fluctuations coherence length in the nematic phase of butylcyano-phenylcyclohexane 312 (1999) 91
- Puzzarini, C., see Aquilanti, V. 318 (2000) 619
- Pyykkö, P., see Kellö, V. 318 (2000) 222
- Qi, F., see Böhmer, R. 316 (2000) 419
- Qian, D., see Sinnott, S.B. 315 (1999) 25
- Qian, S., see Qian, W. 319 (2000) 89
- Qian, W., N.G. Mirkin and S. Krimm, A spectroscopically effective molecular mechanics model for the intermolecular interactions of the hydrogen-bonded *N*-methylacetamide dimer 315 (1999) 125
- Qian, W., L. Lin, Z. Xia, Y. Zou, S. Qian, G. Ma, Y. Lin, R. Cai, Y. Chen and Z.-E. Huang, Measurement of third-order optical nonlinearity of C_{60}M_2 (M = Pd, Pt, and Sm) organometallic compounds by the femtosecond optically heterodyned optical Kerr effect 319 (2000) 89
- Qian, Y., see Lu, Q. 314 (1999) 37
- Qiang, D., see Wang, S. 320 (2000) 411
- Qiao, C., see Zhu, X. 319 (2000) 85
- Qin, Q., see Zhou, M. 318 (2000) 644
- Qin, Q.-Z., see Wang, X. 320 (2000) 144
- Qin, W., see Steinman, E.A. 319 (2000) 1
- Quack, M., see Hippler, M. 314 (1999) 273
- Queralt, J.J., see Sambrano, J.R. 317 (2000) 437
- Quintana, P., see Martínez-Haya, B. 311 (1999) 159
- Quintel, A. and J. Hulliger, A theoretical base for optimising intermolecular interactions driving polarity formation in channel-type host-guest materials 312 (1999) 567

- Quitevis, E.L., J. Martorell, Y. Chang and T.W. Scott, Photoreduction of methylene blue on cadmium sulfide powder 319 (2000) 138
 Quitevis, E.L., see Bryans, T.R. 314 (1999) 459
- Raab, A., On the Dirac-Frenkel/McLachlan variational principle 319 (2000) 674
 Rabin, I., W. Schulze and G. Ertl, Absorption spectra of small silver clusters Ag_n ($n \geq 3$) 312 (1999) 394
 Rabin, I., W. Schulze, G. Ertl, C. Felix, C. Sieber, W. Harbich and J. Buttet, Absorption and fluorescence spectra of Ar-matrix-isolated Ag_3 clusters 320 (2000) 59
 Rabin, I., see Félix, C. 313 (1999) 105
 Radloff, C., see Kelly, K.F. 313 (1999) 445
 Radloff, W., see Farmanara, P. 320 (2000) 697
 Raftery, D., see MacNamara, E. 317 (2000) 165
 Raghavachari, K., see Curtiss, L.A. 313 (1999) 600
 Raghavachari, K., see Curtiss, L.A. 314 (1999) 101
 Rahman, N., see Grossi, G. 313 (1999) 639
 Raimondi, M., see Pelenschikov, A. 314 (1999) 496
 Rakhimov, R.R., H.D. Horton, D.E. Jones, G.B. Loutts and H.R. Ries, Spin dynamics of the triplet Cr^{4+} in the vicinity of energy level anti-crossing 319 (2000) 639
 Rakhmanina, A.V., see Senyavin, V.M. 313 (1999) 421
 Ramsey, M.G., see Duschek, R. 318 (2000) 43
 Randić, M., On characterization of DNA primary sequences by a condensed matrix 317 (2000) 29
 Ranger, M., see Belletête, M. 316 (2000) 101
 Ranke, W., see Joseph, Y. 314 (1999) 195
 Rao, A.M., see Sinnott, S.B. 315 (1999) 25
 Rao, B.K., see Gutsev, G.L. 312 (1999) 598
 Rao, C.N.R., see Mishra, S.R. 317 (2000) 510
 Rao, C.N.R., see Teredesai, P.V. 319 (2000) 296
 Rao, Q., see Xie, R.H. 313 (1999) 211
 Rao, R., T. Sakuntala, S.K. Deb, A.P. Roy, V. Vijayakumar, B.K. Godwal and S.K. Sikka, High-pressure Raman scattering studies on hexamethylenetetramine 313 (1999) 749
 Räsänen, M., see Isoniemi, E. 311 (1999) 47
 Räsänen, M., see Khriachtchev, L. 316 (2000) 115
 Rashev, S., A tier model calculation of the absorption spectrum of the fourth CH stretch overtone state $CH(\nu = 5)$ in benzene 312 (1999) 561
 Rasmussen, A.J. and S.C. Smith, Circulants, symmetry and time-independent wavepacket scattering 312 (1999) 229
 Rasmussen, J.T., M. Hohwy, H.J. Jakobsen and N.C. Nielsen, Magnitude and absolute orientation of 1H chemical shielding tensors in polycrystalline powders: a 1H CRAMPS NMR study of KH_2PO_4 314 (1999) 239
 Rassat, A., G. Del Re and A. Peluso, Neutral mixed-valence organic monoradicals 313 (1999) 582
 Rast, S., see Favier, A. 320 (2000) 49
 Ratajczak, H. and A.M. Yaremko, Theory of the profiles of hydrogen stretching infrared bands of hydrogen-bonded solids. Fermi resonance effect and strong coupling between the high-frequency hydrogen stretching vibration and low-frequency phonons 314 (1999) 122
 Ravikumar, M., Incorporation of temporally correlated internal motions into the magnetic resonance relaxation treatment while considering interference of different relaxation mechanisms 319 (2000) 197
 Ravindra Kumar, G., see Philip, R. 313 (1999) 719

- Rawat, H.S., see Mishra, S.R. 317 (2000) 510
- Rayón, V.M., see Valdés, H. 320 (2000) 507
- Read, F.H., see Mielewska, B. 311 (1999) 428
- Real, J.-A., see Létard, J.-F. 313 (1999) 115
- Real, J.A., see Bousseksou, A. 318 (2000) 409
- Rector, K.D., D.E. Thompson, K. Merchant and M.D. Fayer, Dynamics in globular proteins: vibrational echo experiments 316 (2000) 122
- Reddic, J.E. and M.A. Duncan, Photodissociation spectroscopy of the $\text{Mg}^+-\text{C}_2\text{H}_2$ π -complex 312 (1999) 96
- Redecker, M., see Hofmann, U. 311 (1999) 41
- Redfern, P.C., see Curtiss, L.A. 313 (1999) 600
- Redfern, P.C., see Curtiss, L.A. 314 (1999) 101
- Redondo, J.R., see Redondo, P. 315 (1999) 224
- Redondo, P., J.R. Redondo, C. Barrientos and A. Largo, Theoretical study of the C_3Cl radical and its cation 315 (1999) 224
- Redondo, P., see Barrientos, C. 320 (2000) 481
- Ree, J., see Kim, Y.H. 314 (1999) 1
- Reed, M.A., see Chen, J. 313 (1999) 741
- Refson, K., see Mejias, J.A. 314 (1999) 558
- Regan, P.M., D. Ascenzi, C. Clementi, M.N.R. Ashfold and A.J. Orr-Ewing, The UV photodissociation of HI revisited: REMPI measurements of $\text{I}(^2\text{P})$ atom spin-orbit branching fractions 315 (1999) 187
- Rehbein, C.E.M., see Arnolds, H. 314 (1999) 389
- Rehr, J.J., see Ankudinov, A.L. 316 (2000) 495
- Reid, D.D. and J.M. Wadehra, Scattering of intermediate-energy positrons by C, N, O atoms and the corresponding diatomic molecules: elastic and total cross-sections 311 (1999) 385
- Reid, P.J., see Mayer, S.G. 314 (1999) 246
- Reiher, M., see Andrae, D. 320 (2000) 457
- Reinhardt, P., I. de P.R. Moreira, C. de Graaf, R. Dovesi and F. Illas, Detailed ab-initio analysis of the magnetic coupling in CuF_2 319 (2000) 625
- Reinhold, E., see Scheper, C.R. 312 (1999) 131
- Reinot, T., see Hayes, J.M. 312 (1999) 362
- Reisler, H., see Aristov, V. 318 (2000) 393
- Reiss, D., see Harms, G.S. 313 (1999) 533
- Remko, M. and B.M. Rode, Bivalent cation binding effect on formation of the peptide bond 316 (2000) 489
- Remmers, K., R.G. Satink, G. von Helden, H. Piest, G. Meijer and W.L. Meerts, Gas-phase infrared spectroscopy on the lowest triplet state of the pyrazine-argon complex 317 (2000) 197
- Ren, B., see Xu, X. 311 (1999) 193
- Ren, B., see Cao, P.G. 316 (2000) 1
- Rendell, A.P., see Titmuss, S.J. 320 (2000) 169
- Renge, I., Influence of temperature and pressure on narrow-band fluorescence of 1,8-diphenyloctatetraene in solid crystalline solutions 320 (2000) 373
- Renn, A., see Sepiol, J. 311 (1999) 29
- Renn, A., see Harms, G.S. 313 (1999) 533
- Rentsch, S., see Helbig, M. 312 (1999) 415
- Rentsch, S., see Yang, J.-P. 320 (2000) 665
- Requena, A., see Zúñiga, J. 313 (1999) 670
- Resasco, D.E., see Kitiyanan, B. 317 (2000) 497

- Resch-Genger, U., see Rurack, K. 320 (2000) 87
- Resende, S.M. and F.R. Ornellas, Atmospheric reaction between the HS radical and chlorine 318 (2000) 340
- Ressel, B., see Schmidt, Th. 318 (2000) 549
- Rettig, W. and B. Zietz, Do twisting and pyramidalization contribute to the reaction coordinate of charge-transfer formation in DMABN and derivatives? 317 (2000) 187
- Rettig, W., V. Kharlanov and M. Maus, Excited-state relaxation properties of ionic and nonionic donor-acceptor biphenyl derivatives 318 (2000) 173
- Rettig, W., see Rurack, K. 320 (2000) 87
- Rettig, W., see Van der Meer, M.J. 320 (2000) 673
- Ricca, A., see Bauschlicher, Jr., C.W. 315 (1999) 449
- Rice, C.V., see MacNamara, E. 317 (2000) 165
- Richter, R.C., V.I. Khamaganov and A.J. Hynes, Correlated photofragment product distributions in the photodissociation of NO₂ at 212.8 nm 319 (2000) 341
- Riddell, F.G., see Carter, V.J. 313 (1999) 505
- Rieder, K.-H., see Bartels, L. 313 (1999) 544
- Riedler, M., see Kolmakov, A. 319 (2000) 465
- Riehl, D., see Vivien, L. 312 (1999) 617
- Rienecker, C., see Kolmakov, A. 319 (2000) 465
- Ries, H.R., see Rakhimov, R.R. 319 (2000) 639
- Righi, A., see Alvarez, L. 316 (2000) 186
- Righi, A., see Alvarez, L. 320 (2000) 441
- Ritchie, G.A.D., see Barry, H.R. 319 (2000) 125
- Ritchie, G.L.D., see Lamb, D.W. 317 (2000) 655
- Ritter, M., see Joseph, Y. 314 (1999) 195
- Robbe, J.M., see Cossart, D. 311 (1999) 248
- Roberts, G., see Arnolds, H. 314 (1999) 389
- Robertson, S.H., see Green, N.J.B. 314 (1999) 376
- Robinson, A.P.G., R.E. Palmer, T. Tada, T. Kanayama, E.J. Shelley, D. Philp and J.A. Preece, Exposure mechanism of fullerene derivative electron beam resists 312 (1999) 469
- Robinson, G.H., see Xie, Y. 317 (2000) 174
- Rocha, W.R., K.J. De Almeida and W.B. De Almeida, Liquid tin tetrachloride: a Monte Carlo simulation study 316 (2000) 510
- Rode, B.M., see Remko, M. 316 (2000) 489
- Rode, M., J. Sadlej, R. Moszynski, P.E.S. Wormer and A. Van der Avoird, The importance of high-order correlation effects for the CO-CO interaction potential 314 (1999) 326
- Rodríguez, A., see Alvarino, J.M. 313 (1999) 299
- Rohmund, F., see Nikolaev, P. 313 (1999) 91
- Roitberg, A., see Markelz, A.G. 320 (2000) 42
- Rolla, P.A., see Corezzi, S. 320 (2000) 113
- Rols, S., see Alvarez, L. 316 (2000) 186
- Rols, S., see Alvarez, L. 320 (2000) 441
- Romanini, D., see Booth, J.P. 317 (2000) 633
- Roos, B.O., see Gagliardi, L. 320 (2000) 518
- Rosenwaks, S., see Melchior, A. 315 (1999) 421
- Rosmus, P., see Panten, D. 311 (1999) 390
- Rossi, L., see Ariu, M. 313 (1999) 405
- Rossky, P.J., see Turi, L. 316 (2000) 465

- Roszak, S., R. Gora and J. Leszczynski, A theoretical study of the structures and energetics of O^-Ar_n ($n = 1-6$) clusters 313 (1999) 198
- Roszak, S. and J. Leszczynski, The structures, thermodynamics, and nature of interactions of silanium cations shellvated by molecular hydrogen, $SiH_3^+(H_2)_n$ ($n = 1-11$) 314 (1999) 333
- Rourke, D.E., see Bush, S.D. 311 (1999) 379
- Rousseau, E., see Jin, Y.D. 320 (2000) 387
- Rowlen, K.L., see Simpson, G.J. 317 (2000) 276
- Roy, A.P., see Rao, R. 313 (1999) 749
- Rozas, I., see Alkorta, I. 311 (1999) 281
- Rubahn, H.-G., see Boneß, J. 313 (1999) 19
- Rubio, A., see Boustani, I. 311 (1999) 21
- Rubner, O., T. Baumert, M. Bergt, B. Kiefer, G. Gerber and V. Engel, Theoretical analysis of femtosecond excitation and fragmentation dynamics of $Fe(CO)_5$ 316 (2000) 585
- Rudavets, M.G., see Fel'dman, E.B. 311 (1999) 453
- Rudić, S., see Labazan, I. 320 (2000) 613
- Rueda-Morales, G., see Venegas, V. 318 (2000) 655
- Ruhman, S., see Wang, Z. 313 (1999) 155
- Ruhman, S., see Ye, T. 314 (1999) 429
- Ruhstaller, B., J.C. Scott, P.J. Brock, U. Scherf and S.A. Carter, Bias-tuned reduction of self-absorption in polymer blend electroluminescence 317 (2000) 238
- Rupp, W., see Foltynowicz, R.J. 315 (1999) 210
- Rurack, K., M. Szczepan, M. Spieles, U. Resch-Genger and W. Rettig, Correlations between complex stability and charge distribution in the ground state for Ca^{II} and Na^I complexes of charge transfer chromo- and fluoroionophores 320 (2000) 87
- Ruscic, B. and M. Litorja, Photoionization of HOCO revisited: a new upper limit to the adiabatic ionization energy and lower limit to the enthalpy of formation 316 (2000) 45
- Russell, D.M., see Silva, C. 319 (2000) 494
- Russo, M.V., see Casalboni, M. 319 (2000) 107
- Rustagi, K.C., see Mishra, S.R. 317 (2000) 510
- Rustici, M., see Marchettini, N. 317 (2000) 649
- Rutigliano, M., see Bruno, D. 320 (2000) 245
- Ruud, K., see Polavarapu, P.L. 319 (2000) 595
- Ryabov, E.A., see Dem'yanenko, A.V. 320 (2000) 594
- Rychlewski, J., see Cioslowski, J. 319 (2000) 542
- Rychlewski, J., see Cencek, W. 320 (2000) 549
- Ryjáček, F., M. Kratochvíl and P. Hobza, Adenine \cdots 2,4-difluorotoluene (modified base) pair: potential and free-energy surfaces. Non-empirical and empirical potential studies 313 (1999) 393
- Saalfrank, P., see Bartels, L. 313 (1999) 544
- Saalfrank, P., see Nest, M. 313 (1999) 665
- Sachse, T.I., K.T. Tang and J.P. Toennies, A simple damping function for the three-atom dispersion energy 317 (2000) 346
- Sadlej, A.J., see Jankowski, K. 311 (1999) 265
- Sadlej, A.J., see Ingamells, V.E. 316 (2000) 541
- Sadlej, A.J., see Kellö, V. 318 (2000) 222
- Sadlej, J., see Rode, M. 314 (1999) 326
- Sadlej, J., see Myszkiewicz, G. 318 (2000) 232

- Safont, V.S., M. Oliva, J. Andrés and O. Tapia, Alternative pathways for the C2–C3 bond cleavage and C2 configuration inversion processes for the Rubisco-catalyzed carboxylation sequence 318 (2000) 361
- Sagdeev, R.Z., see Makarov, T.N. 317 (2000) 252
- Sagon, G., see Senyavin, V.M. 313 (1999) 421
- Saini, R.D., see Dhanya, S. 318 (2000) 125
- Sainov, N.A., see Kukovitsky, E.F. 317 (2000) 65
- Saito, K., M. Okada, H. Akutsu and M. Sorai, Can the molecule involved in a CT interaction reorient itself in the crystal lattice? Phase transition and glass transition in *trans*-stilbene-TCNQ 318 (2000) 75
- Saito, K., see Kato, N. 312 (1999) 115
- Saitow, K., see Nakayama, H. 320 (2000) 323
- Sakabe, S., see Shimizu, S. 317 (2000) 611
- Sakaguchi, K., see Kikuchi, K. 319 (2000) 472
- Sakai, M., see Mitsui, M. 317 (2000) 211
- Sakai, S., Theoretical study on the photochemical reactions of butadiene, cyclobutene and bicyclobutane 319 (2000) 687
- Sakashita, M., see Nakayama, H. 320 (2000) 323
- Sakata, K. and A. Tachibana, Quantum-chemical study on the reaction between GeF_4 and Si_2H_6 320 (2000) 527
- Sakata, T., see Ohtake, T. 318 (2000) 517
- Sakellariou, D., A. Lesage, P. Hodgkinson and L. Emsley, Homonuclear dipolar decoupling in solid-state NMR using continuous phase modulation 319 (2000) 253
- Sakuntala, T., see Rao, R. 313 (1999) 749
- Sakuragi, H., see Hashimoto, J. 314 (1999) 261
- Salafsky, J.S. and K.B. Eisenthal, Second harmonic spectroscopy: detection and orientation of molecules at a biomembrane interface 319 (2000) 435
- Salamon, M., see Maruszewski, K. 314 (1999) 83
- Salin, A., see Busnengo, H.F. 320 (2000) 328
- Salsi, L.D., see Vincent, M.A. 314 (1999) 138
- Salzborn, E., see Hathiramani, D. 319 (2000) 13
- Sambrano, J.R., A.R. de Souza, J.J. Queralto and J. Andrés, A theoretical study on cytosine tautomers in aqueous media by using continuum models 317 (2000) 437
- Samoilova, R.I., A.A. Shubin, M.K. Bowman, J. Hüttermann and S.A. Dikanov, Observation of two paramagnetic species in electron transfer reactions within cesium modified X and Y zeolites 316 (2000) 404
- Sancho-García, J.C., A.J. Pérez-Jiménez and F. Moscardó, A comparison between DFT and other ab initio schemes on the activation energy in the automerization of cyclobutadiene 317 (2000) 245
- Sancho-García, J.C. and A.J. Pérez-Jiménez, A systematic and accurate study of singlet propynylidene 318 (2000) 649
- Sanekata, M. and I. Suzuka, Optical absorptions of the X-center-type sodium nanoclusters in the gas-aggregation technique with a reactant nozzle 312 (1999) 422
- San Fabián, J., see Guilleme, J. 314 (1999) 168
- Sanov, A., J. Faeder, R. Parson and W.C. Lineberger, Spin-orbit coupling in $\text{I} \cdot \text{CO}_2$ and $\text{I} \cdot \text{OCS}$ van der Waals complexes: beyond the pseudo-diatomic approximation 313 (1999) 812
- Santamaría, J., see Martínez-Haya, B. 311 (1999) 159
- Santra, S., G. Krishnamoorthy and S.K. Dogra, Excited state intramolecular proton transfer in 2-(2'-benzamido-phenyl)benzimidazole: effect of solvents 311 (1999) 55

- Sanyal, S., see Sethia, A. 315 (1999) 299
- Sapre, A.V., see Bhasikuttan, A.C. 316 (2000) 67
- Sarcinelli, F., see Casalboni, M. 319 (2000) 107
- Sarobe, M., R.H. Fokkens, T.J. Cleij, L.W. Jenneskens, N.M.M. Nibbering, W. Stas and C. Versluis, S_8 -mediated cyclotrimerization of 4,5-dihydrobenz[1]acephenanthrylene: trinaphthodecacyclene ($C_{60}H_{30}$) isomers and their propensity towards cyclodehydrogenation 313 (1999) 31
- Saß, M., J. Löbau, M. Lettenberger and A. Laubereau, Vibrational energy transfer of chemisorbed ethyltrichlorosilane at the glass/air interface 311 (1999) 13
- Sathyamurthy, N., see Abrol, R. 312 (1999) 341
- Sathyamurthy, N., see Maheshwari, S. 315 (1999) 181
- Satink, R.G., see Remmers, K. 317 (2000) 197
- Sato, K., see Takayanagi, T. 312 (1999) 503
- Sato, K., see Kohno, M. 319 (2000) 451
- Sato, T., see Nakano, T. 318 (2000) 614
- Sato, Y., see Ohmori, K. 315 (1999) 411
- Satoh, G., see Ichikawa, T. 313 (1999) 129
- Satoh, K. and S. Iwata, Theoretical study of vibrational spectra for $Cl^-(H_2O)$: temperature dependence and the influence of Ar_n ($n = 1-3$) 312 (1999) 522
- Satta, M., A. Latini, S. Piccirillo, T.M. Di Palma, D. Scuderi, M. Speranza and A. Giardini, Energetics of monohydrated chiral R(+)-1-phenyl-1-propanol: supersonic beam experiments and density functional calculations 316 (2000) 94
- Sattigeri, J.A., see Hsu, C.-C. 311 (1999) 355
- Sattler, K., see Lonfat, M. 313 (1999) 539
- Sauer, J., see Vener, M.V. 312 (1999) 591
- Sauvajol, J.-L., see Alvarez, L. 316 (2000) 186
- Sauvajol, J.L., see Alvarez, L. 320 (2000) 441
- Savitsky, A.N. and H. Paul, Reversed triplet mechanism CIDEP in triplet azoalkanes 319 (2000) 403
- Sawada, T., see Ito, K. 318 (2000) 1
- Sawai, T., see Kitaura, K. 312 (1999) 319
- Scandola, F., see Borsarelli, C.D. 317 (2000) 53
- Scarano, D., see Wolter, K. 320 (2000) 206
- Schaak, A., see Schmidt, Th. 318 (2000) 549
- Schaefer III, H.F., see Xie, Y. 317 (2000) 174
- Schaer, M., see Donzé, N. 315 (1999) 405
- Schäfer, J., A. Simons, J. Wolfrum and R.A. Fischer, Detection of gas-phase species in MOCVD of GaN using molecular beam quadrupole mass spectrometry 319 (2000) 477
- Schaffner, K., see Kneip, C. 311 (1999) 479
- Schastnev, P.V., see Shchegoleva, L.N. 312 (1999) 325
- Schatz, G.C., see Ishida, T. 314 (1999) 369
- Scheblykin, I.G., M.M. Bataiev, M. Van der Auweraer and A.G. Vitukhnovsky, Dimensionality and temperature dependence of the radiative lifetime of J-aggregates with Davydov splitting of the exciton band 316 (2000) 37
- Scheer, H., see Fiedor, L. 319 (2000) 145
- Scheffler, M., see Eichler, A. 311 (1999) 1
- Scheier, P., see Hathiramani, D. 319 (2000) 13
- Scheller, D., see Fedurco, M. 319 (2000) 309

- Scheper, C.R., C.A. De Lange, A. De Lange, E. Reinhold and W. Ubachs, Dissociation of H_2 in the energy region at the $H(n=1) + H(n=3)$ dissociation threshold after $(1 + 1')$ resonance-enhanced two-photon ionization via the $B^1\Sigma_u^+$ state 312 (1999) 131
- Scherf, U., see Wegmann, G. 312 (1999) 376
- Scherf, U., see Schweitzer, B. 313 (1999) 57
- Scherf, U., see Harrison, M.G. 313 (1999) 755
- Scherf, U., see Ruhstaller, B. 317 (2000) 238
- Schilling, M., see Mirau, P.A. 313 (1999) 139
- Schinke, R., see Klossika, J.-J. 314 (1999) 182
- Schmeißer, D., see Appel, G. 313 (1999) 411
- Schmickler, W., A theory for nonadiabatic electrochemical electron-transfer reactions involving the breaking of a bond 317 (2000) 458
- Schmickler, W., see Leiva, E.P.M. 320 (2000) 393
- Schmider, H.L., see Jin, B. 317 (2000) 464
- Schmidt, J., see Durand, Y. 317 (2000) 232
- Schmidt, K. and M. Springborg, Comment on: "Relativistic all-electron Hartree-Fock-Dirac calculation of a quasi one-dimensional chain of selenium atoms" 320 (2000) 1
- Schmidt, Th., A. Schaak, S. Günther, B. Ressel, E. Bauer and R. Imbihl, In situ imaging of structural changes in a chemical wave with low-energy electron microscopy: the system $Rh(110)/NO + H_2$ 318 (2000) 549
- Schnabel, W., see Naik, D.B. 315 (1999) 416
- Schneider, C., see Potrzebowski, M.J. 313 (1999) 569
- Schneider, F.W., see Guderian, A. 312 (1999) 440
- Schneider, F.W., see Fecher, F. 313 (1999) 205
- Schnitzer, C., S. Baldelli and M.J. Shultz, Sum frequency generation by water on supercooled H_2SO_4/H_2O liquid solutions at stratospheric temperature 313 (1999) 416
- Schott, M., see Lécuyer, R. 314 (1999) 255
- Schreiber, A., see Hofmann, U. 311 (1999) 41
- Schreiber, M., see Nest, M. 313 (1999) 665
- Schröder, D., see Srinivas, R. 316 (2000) 243
- Schulze, W., see Rabin, I. 312 (1999) 394
- Schulze, W., see Félix, C. 313 (1999) 105
- Schulze, W., see Rabin, I. 320 (2000) 59
- Schütz, M. and H.-J. Werner, Local perturbative triples correction (T) with linear cost scaling 318 (2000) 370
- Schwartz, R.W., see Marcus, R.K. 318 (2000) 481
- Schwarz, H., see Srinivas, R. 316 (2000) 243
- Schweig, A., see Gödicke, B. 318 (2000) 102
- Schweitzer, B., V.I. Arkhipov, U. Scherf and H. Bässler, Geminate pair recombination in a conjugated polymer 313 (1999) 57
- Schweitzer, B., see Wegmann, G. 312 (1999) 376
- Schwenke, D.W., see Tyuterev, V.I.G. 316 (2000) 271
- Schwerdtfeger, P., see Pernpointner, M. 316 (2000) 141
- Schwerdtfeger, P., see Kellö, V. 318 (2000) 222
- Schwerdtfeger, P., see Seth, M. 318 (2000) 314
- Scott, C.D., see Iliev, M.N. 316 (2000) 217
- Scott, C.D., see Arepalli, S. 320 (2000) 26
- Scott, J.C., see Ruhstaller, B. 317 (2000) 238

- Scott, T.W., see Quitevis, E.L. 319 (2000) 138
- Scuderi, D., see Satta, M. 316 (2000) 94
- Scuseria, G.E., see Jaramillo, J. 312 (1999) 269
- Scuseria, G.E., see Kelly, K.F. 313 (1999) 445
- Sczegan, M., see Rurack, K. 320 (2000) 87
- Sears, T.J., see Steimle, T.C. 319 (2000) 363
- Secombe, D.P., see Jarvis, G.K. 315 (1999) 287
- Segawa, K., see Hashimoto, J. 314 (1999) 261
- Sehested, K., see Wallington, T.J. 313 (1999) 456
- Seibold, M., H. Port and K. Gustav, Determination of reaction quantum yields of photochromic fulgides using mid-IR spectroscopy: quantitative evaluation and normal mode analysis 314 (1999) 65
- Seifert, G. and E. Hernández, Theoretical prediction of phosphorus nanotubes 318 (2000) 355
- Seifert, G., see Heine, T. 316 (2000) 373
- Seki, K., see Ochimizu, T. 313 (1999) 451
- Sekiya, A., see Chandra, A.K. 318 (2000) 69
- Sekkat, Z., see Ishitobi, H. 316 (2000) 578
- Selvan, R., R. Unnikrishnan, S. Ganapathy and T. Pradeep, Macroscopic synthesis and characterization of giant fullerenes 316 (2000) 205
- Semkin, V.N., see Konarev, D.V. 314 (1999) 570
- Sen, R., see Teredesai, P.V. 319 (2000) 296
- Sensui, N., see Yudasaka, M. 312 (1999) 155
- Senyavin, V.M., V.A. Davydov, L.S. Kashevarova, A.V. Rakhmanina, V. Agafonov, H. Allouchi, R. Céolin, G. Sagon and H. Szwarc, Spectroscopic properties of individual pressure-polymerized phases of C₆₀ 313 (1999) 421
- Seong, J., K.C. Janda, M.P. McGrath and N. Halberstadt, HeNe⁺: resolution of an apparent disagreement between experiment and theory 314 (1999) 501
- Sepiol, J., A. Starukhin, R. Kolos, T. Lutychevskaia, J. Jasny, A. Renn and U.P. Wild, Detection and spectroscopy of single molecules in rare gas matrices: dibenzanthanthrene in krypton and xenon 311 (1999) 29
- Serebryanaya, N.R., see Chernozatonskii, L.A. 316 (2000) 199
- Sergenton, A.-C. and M. Allan, Excitation of vibrational levels of HI up to $v = 8$ by electron impact 319 (2000) 179
- Serra, P. and S. Kais, Data collapse for the Schrödinger equation 319 (2000) 273
- Seta, P., see Konstantaki, M. 318 (2000) 488
- Setayesh, S., see Silva, C. 319 (2000) 494
- Seth, M. and P. Schwerdtfeger, A comparison of relativistic and electron correlation effects for (111)F, (111)H and (111)Li 318 (2000) 314
- Sethia, A., S. Sanyal and F. Hirata, Eigenstates from the discretized path integral 315 (1999) 299
- Setser, D.W., see Butkovskaya, N.I. 312 (1999) 37
- Sette, M., see Capuani, S. 316 (2000) 222
- Sha, G.H., see Chen, X.L. 318 (2000) 107
- Shafizadeh, N., see Campos, A. 314 (1999) 91
- Shaik, S., see Filatov, M. 316 (2000) 135
- Shakirov, S.R., see Makarov, T.N. 317 (2000) 252
- Shalashilin, D.V. and B. Jackson, Guiding paths and time-dependent basis sets for wavefunction propagation 318 (2000) 305

- Shao, X.-G., see Cai, W.-S. 319 (2000) 708
- Shapovalov, V., T.N. Truong, A. Kovalenko and F. Hirata, Liquid structure at metal oxide–water interface: accuracy of a three-dimensional RISM methodology 320 (2000) 186
- Shchegoleva, L.N., I.V. Beregovaya and P.V. Schastnev, Potential energy surface of $C_6F_6^-$ radical anion 312 (1999) 325
- Shelley, E.J., see Robinson, A.P.G. 312 (1999) 469
- Sheves, M., see Ye, T. 314 (1999) 429
- Shevtsov, V., T. Kumada, Y. Aratono and T. Miyazaki, The pressure effect on the recombination and relaxation of hydrogen atoms in solid hydrogen 319 (2000) 535
- Shi, Y. and K.M. Ervin, Gas-phase acidity and C–H bond energy of diacetylene 318 (2000) 149
- Shi, Y.-R., see Wei, T.-X. 319 (2000) 7
- Shi, Z., see Wang, S. 320 (2000) 411
- Shiau, C.-W., see Hsu, C.-C. 311 (1999) 355
- Shiell, R.C., M. Evans, S. Stimson, C.-W. Hsu, C.Y. Ng and J.W. Hepburn, A ZEKE photoelectron study of the $D^2\Pi$ and $3^2\Sigma^+$ satellite states of CO^+ 315 (1999) 390
- Shigeiwa, M., see Myers, D.J. 312 (1999) 399
- Shigeiwa, M., see Myers, D.J. 313 (1999) 592
- Shigeta, Y., T. Kawakami, H. Nagao and K. Yamaguchi, A theoretical study of spin level crossing induced by an external magnetic field of ring molecule magnet models 315 (1999) 441
- Shigeta, Y., see Soda, T. 319 (2000) 223
- Shim, I. and K.A. Gingerich, All-electron ab initio investigations of the three lowest-lying electronic states of the RuC molecule 317 (2000) 338
- Shimizu, A. and H. Tachikawa, A direct molecular orbital dynamics study on proton transfer in the diamond lattice 314 (1999) 516
- Shimizu, K., see Shimizu, S. 317 (2000) 611
- Shimizu, S., J. Kou, S. Kawato, K. Shimizu, S. Sakabe and N. Nakashima, Coulomb explosion of benzene irradiated by an intense femtosecond laser pulse 317 (2000) 611
- Shimobe, Y., see Mukai, K. 311 (1999) 446
- Shimomura, S., see Yamaguchi, Y. 316 (2000) 477
- Shin, H.K., see Kim, Y.H. 314 (1999) 1
- Shin, S.K., see Son, H.S. 320 (2000) 658
- Shin, Y.B., J. Heo and H.S. Kim, Modification of the local phonon modes and electron–phonon coupling strengths in Dy^{3+} -doped sulfide glasses for efficient 1.3 μm amplification 317 (2000) 639
- Shinohara, H., see Okazaki, T. 320 (2000) 435
- Shiotani, M., see Harima, Y. 317 (2000) 310
- Shiotani, M., see Wang, P. 320 (2000) 623
- Shiratori, H., T. Ohno, K. Nozaki and A. Osuka, Coordination control of intramolecular energy transfer in boronate-bridged naphthalene-aryl ketone molecule 320 (2000) 631
- Shoute, L.C.T., see Pan, D. 316 (2000) 395
- Shramek, N.S., see Ishikawa, Y. 313 (1999) 341
- Shrivastava, K.N., S.S.C. Ammal, H. Tsuruya, S. Takami, A. Endou, M. Kubo, K. Teraishi, A. Miyamoto and A. Ozaki, Density functional theory calculations of molecular nitrogen on a ruthenium cluster 313 (1999) 279
- Shubin, A.A., see Samoilova, R.I. 316 (2000) 404
- Shultz, M.J., see Schnitzer, C. 313 (1999) 416
- Shushin, A.I., Detailed analysis of the mechanism of net electron spin polarization in liquid phase triplet-radical quenching 313 (1999) 246

- Shvartsburg, A.A. and M.F. Jarrold, Transition from covalent to metallic behavior in group-14 clusters 317 (2000) 617
- Siddiqui, S., see Spano, F.C. 314 (1999) 481
- Sidis, V., see Babikov, D. 316 (2000) 129
- Sieber, C., see Félix, C. 313 (1999) 105
- Sieber, C., see Rabin, I. 320 (2000) 59
- Siebrand, W. and M.Z. Zgierski, Theoretical study of the excited-state proton-transfer threshold in 1-naphthol-ammonia complexes 320 (2000) 153
- Signorell, R., M. Somavilla and F. Merkt, Jahn-Teller distortion in $CD_2H_2^+$ from a rotationally resolved photoelectron spectrum 312 (1999) 139
- Sikka, S.K., see Rao, R. 313 (1999) 749
- Silbey, R., see Myers, D.J. 312 (1999) 399
- Sildos, I., see Babin, V. 314 (1999) 31
- Silva, C., D.M. Russell, M.A. Stevens, J.D. Mackenzie, S. Setayesh, K. Müllen and R.H. Friend, Excited-state absorption in luminescent conjugated polymer thin films: ultrafast studies of processable polyindenofluorene derivatives 319 (2000) 494
- Silverans, R.E., see Bouwen, W. 314 (1999) 227
- Sim, W.S., see Zou, Z. 312 (1999) 149
- Simas, A.M., see Ventura, E. 320 (2000) 587
- Siminovitch, D., see Jarrell, H.C. 314 (1999) 421
- Simon, B., see Maurin, G. 312 (1999) 14
- Simón-Manso, Y., see Fuentealba, P. 314 (1999) 108
- Simons, A., see Schäfer, J. 319 (2000) 477
- Simpson, C.J.S.M., see Griffiths, P.T. 315 (1999) 158
- Simpson, G.J. and K.L. Rowlen, Influence of substrate roughness on orientation measurements by second-harmonic generation 317 (2000) 276
- Sin, J.M., see Soos, Z.G. 319 (2000) 631
- Sinclair, W.E., see Pfluger, D. 313 (1999) 171
- Sinisterra, R.D., see Dos Santos, H.F. 319 (2000) 569
- Sinnott, S.B., R. Andrews, D. Qian, A.M. Rao, Z. Mao, E.C. Dickey and F. Derbyshire, Model of carbon nanotube growth through chemical vapor deposition 315 (1999) 25
- Sironi, M., see Pelmenchikov, A. 314 (1999) 496
- Siu, C.K., see Liu, Z.F. 311 (1999) 93
- Siu, C.K., see Liu, Z.F. 314 (1999) 317
- Sizova, O.V., see Baranovski, V.I. 315 (1999) 130
- Sizun, M., see Babikov, D. 316 (2000) 129
- Skenderović, H., see Ban, T. 313 (1999) 110
- Skinner, J.L., see Egorov, S.A. 317 (2000) 560
- Skokov, S., K.A. Peterson and J.M. Bowman, Perturbative inversion of the HOCl potential energy surface via singular value decomposition 312 (1999) 494
- Skokov, S., see Christoffel, K.M. 315 (1999) 275
- Skourtis, S.S., see Xie, Q. 312 (1999) 237
- Škrinářová, Z., K. Bowden and W.M.F. Fabian, An ab initio and density functional study on the ring-chain tautomerism of (Z)-3-formyl-acrylic acid 316 (2000) 531
- Sloan, J., R.E. Dunin-Borkowski, J.L. Hutchison, K.S. Coleman, V.C. Williams, J.B. Claridge, A.P.E. York, C. Xu, S.R. Bailey, G. Brown, S. Friedrichs and M.L.H. Green, The size distribution, imaging and obstructing properties of C_{60} and higher fullerenes formed within arc-grown single walled carbon nanotubes 316 (2000) 191

- Sluiter, M., see Belosludov, R.V. 312 (1999) 299
- Small, G.J., see Hayes, J.M. 312 (1999) 362
- Smalley, R.E., see Nikolaev, P. 313 (1999) 91
- Smalley, R.E., see Arepalli, S. 320 (2000) 26
- Smeijja, J.A., see Gilbert, D.C. 315 (1999) 43
- Smith, B.W., M. Monthieux and D.E. Luzzi, Carbon nanotube encapsulated fullerenes: a unique class of hybrid materials 315 (1999) 31
- Smith, J., see MacNamara, E. 317 (2000) 165
- Smith, K.A., see Nikolaev, P. 313 (1999) 91
- Smith, L.J., see MacNamara, E. 317 (2000) 165
- Smith, S.C., see Rasmussen, A.J. 312 (1999) 229
- Snijders, J.G., see de Lange, M.J.L. 313 (1999) 491
- Snyder, J.A. and E.D. Stevens, A wavefunction and energy of the azide ion in potassium azide obtained by a quantum-mechanically constrained fit to X-ray diffraction data 313 (1999) 293
- So, S.P., A Gaussian-2 molecular orbital study of the reaction of CF_3 with NO_2 313 (1999) 307
- So, S.P., Theoretical study of Si_3H_3^+ and Ge_3H_3^+ isomers 313 (1999) 587
- Soave, R. and G. Pacchioni, New bonding mode of CO on stepped MgO surfaces from density functional cluster model calculations 320 (2000) 345
- Sobolewski, A.L. and W. Domcke, Ab initio investigations on the photophysics of indole 315 (1999) 293
- Soda, T., Y. Kitagawa, T. Onishi, Y. Takano, Y. Shigeta, H. Nagao, Y. Yoshioka and K. Yamaguchi, Ab initio computations of effective exchange integrals for H-H, H-He-H and Mn_2O_2 complex: comparison of broken-symmetry approaches 319 (2000) 223
- Sokalski, W.A., see Grembecka, J. 313 (1999) 385
- Sokolova, S. and A. Luchow, An ab initio study of TiC with the diffusion quantum Monte Carlo method 320 (2000) 421
- Sokolowski, D., J.F. Castillo and C. Tully, Semiclassical angular scattering in the $\text{F} + \text{H}_2 \rightarrow \text{HF} + \text{H}$ reaction: Regge pole analysis using the Padé approximation 313 (1999) 225
- Sokolowski, M., see Hopmeier, M. 314 (1999) 9
- Solanki, N.K., see Bridgeman, A.J. 314 (1999) 176
- Soldán, P., E.P.F. Lee, S.D. Gamblin and T.G. Wright, Structure and stability of the $\text{Na}^+ \cdot \text{CO}_2$ and $\text{Na}^+ \cdot \text{H}_2\text{O}$ complexes 313 (1999) 379
- Solntsev, K.M. and N. Agmon, Dual asymptotic behavior in geminate diffusion-influenced reaction 320 (2000) 262
- Sommavilla, M., see Signorell, R. 312 (1999) 139
- Son, H.S., K. Lee, S.K. Shin and J.K. Ku, Radiative lifetimes of the FeO orange system 320 (2000) 658
- Song, M.-B., see Nakamura, M. 320 (2000) 381
- Song, X., see Bu, Y. 319 (2000) 725
- Sonoyama, N., see Ohtake, T. 318 (2000) 517
- Sood, A.K., see Mishra, S.R. 317 (2000) 510
- Sood, A.K., see Teredesai, P.V. 319 (2000) 296
- Soos, Z.G., S. Bao, J.M. Sin and G.W. Hayden, Compensation temperature in molecularly doped polymers 319 (2000) 631
- Sorai, M., see Saito, K. 318 (2000) 75
- Sordo, J.A., On the important role played by polarization functions in calculations involving hypervalent molecules 316 (2000) 167
- Sordo, J.A., see Valdés, H. 320 (2000) 507
- Spadacini, R., see Ferrando, R. 315 (1999) 153
- Spano, F.C. and S. Siddiqui, Exciton-vibrational coupling in pinwheel aggregates of π -conjugated molecules 314 (1999) 481

- Speranza, M., see Satta, M. 316 (2000) 94
- Spieles, M., see Rurack, K. 320 (2000) 87
- Springborg, M., see Schmidt, K. 320 (2000) 1
- Srinivas, R., S. Vivekananda, D. Schröder and H. Schwarz, SiNCO^+ and SiNCS^+ and their neutral counterparts 316 (2000) 243
- St-Amant, A., see Archibong, E.F. 316 (2000) 151
- Stachó, L.L., G. Dömötör and M.I. Bán, On the Elber–Karplus reaction path-following method and related procedures 311 (1999) 328
- Stagira, S., see Lanzani, G. 313 (1999) 525
- Starukhin, A., see Sepiol, J. 311 (1999) 29
- Starukhin, A., see Dobkowski, J. 318 (2000) 79
- Stas, W., see Sarobe, M. 313 (1999) 31
- Steimle, T.C., M.L. Costen, G.E. Hall and T.J. Sears, Transient frequency modulation absorption spectroscopy of molecules produced in a laser ablation supersonic expansion source 319 (2000) 363
- Steiner, U.E., see Fodor, L. 316 (2000) 411
- Steinman, E.A., V.V. Kveder, D.V. Konarev, W. Qin and H.G. Grimmeiss, Charge transfer state of novel molecular complex $\text{C}_{26}\text{H}_{18}\text{Te}_2 \cdot \text{C}_{60} \cdot \text{CS}_2$ detected in single crystals by photoluminescence and ESR 319 (2000) 1
- Stepanenko, Y., see Nosenko, Y. 315 (1999) 87
- Stephan, C., see Colomer, J.-F. 317 (2000) 83
- Stephens, A.D., see Mattar, S.M. 319 (2000) 601
- Stert, V., see Farmanara, P. 320 (2000) 697
- Stevens, E.D., see Snyder, J.A. 313 (1999) 293
- Stevens, M.A., see Silva, C. 319 (2000) 494
- Stichler, M., see Föhlich, A. 315 (1999) 194
- Stimson, S., see Shiell, R.C. 315 (1999) 390
- Stöckle, R.M., Y.D. Suh, V. Deckert and R. Zenobi, Nanoscale chemical analysis by tip-enhanced Raman spectroscopy 318 (2000) 131
- Stoll, H., see Albrecht, M. 319 (2000) 355
- Stolte, S., see de Lange, M.J.L. 313 (1999) 491
- Stolte, S., see Griffiths, P.T. 315 (1999) 158
- Stoyanov, N., see Enchev, V. 314 (1999) 234
- Strasser, J., see Homeier, H.H.H. 316 (2000) 280
- Strasser, P., see Fecher, F. 313 (1999) 205
- Strazisar, B.R., see Bernard, E.J. 313 (1999) 461
- Strehle, M., see Frohmeyer, T. 312 (1999) 447
- Streiff, J.H., W.D. Edwards and J.L. McHale, Investigation of the solvatochromic electronic transitions of $[\text{Ru}(\text{NH}_3)_4\text{bipyridine}]^{2+}$ 312 (1999) 369
- Stręk, W., see Maruszewski, K. 314 (1999) 83
- Stry, S., see Kleine, D. 312 (1999) 185
- Styszyński, J., Relativistic core–valence correlation effects on molecular properties of the hydrogen halide molecules 317 (2000) 351
- Su, K., see Wang, Y. 312 (1999) 277
- Su, M.-C., see Michael, J.V. 319 (2000) 99
- Su, M.-D. and S.-Y. Chu, Theoretical study of geometrical effect on the deoxygenation of epoxide by singlet carbenes 320 (2000) 475
- Sueki, K., see Akiyama, K. 317 (2000) 490

- Sueki, K., see Kikuchi, K. 319 (2000) 472
- Suenaga, K., M. Yudasaka, C. Colliex and S. Iijima, Radially modulated nitrogen distribution in CN_x nanotubular structures prepared by CVD using Ni phthalocyanine 316 (2000) 365
- Suenaga, K., see Okazaki, T. 320 (2000) 435
- Suenram, R.D., see McIntosh, A. 314 (1999) 57
- Sugai, Y., see Kinoshita, M. 313 (1999) 685
- Sugawara, M., Adaptive basis set for quantum-mechanical calculation based on element-free Galerkin method 314 (1999) 522
- Sugawara, T., see Nakazaki, J. 319 (2000) 385
- Sugie, M., see Chandra, A.K. 318 (2000) 69
- Sugita, Y. and Y. Okamoto, Replica-exchange molecular dynamics method for protein folding 314 (1999) 141
- Suh, Y.D., see Stöckle, R.M. 318 (2000) 131
- Suits, A.G., see Peterka, D.S. 312 (1999) 108
- Suits, A.G., see Ahmed, M. 317 (2000) 264
- Sukul, D., see Pal, S.K. 312 (1999) 178
- Suleimenov, O., see Ha, T.-K. 315 (1999) 327
- Sulkes, M., L.C. Baldwin and M.J. Fink, Molecular beam study of possible CVD intermediates from Group-14 organometallic precursors 318 (2000) 448
- Sumiyoshi, Y., see Tang, J. 315 (1999) 69
- Sumpter, B.G., see Ford, J.V. 316 (2000) 181
- Sumpter, B.G., see Noid, D.W. 316 (2000) 285
- Sun, C.-C., see Yu, X. 320 (2000) 123
- Sun, C.C., see Lu, W.C. 311 (1999) 491
- Sun, X., see Jin, Z. 318 (2000) 505
- Sun, X.H., see Cheng, L.F. 319 (2000) 418
- Sun, Y., see Sun, Z. 318 (2000) 471
- Sun, Y.-C., H.-F. Lu and M.-S. Ho, Molecular dynamics simulation of hydrogen isotope-terminated silicon(111) and (110) surfaces: calculation of vibrational energy relaxation rates of hydrogen isotope stretching modes 318 (2000) 7
- Sun, Z., Y. Sun and X. Wang, Investigation of phases in the carbon films deposited by electrolysis of ethanol liquid phase using Raman scattering 318 (2000) 471
- Sun, Z., see Zhu, X. 319 (2000) 85
- Sundermann, K., see Andrianov, I. 318 (2000) 256
- Sundholm, D., Density functional theory study of the electronic absorption spectrum of Mg-porphyrin and Mg-etioporphyrin-I 317 (2000) 392
- Sundholm, D., Comparison of the electronic excitation spectra of chlorophyll *a* and pheophytin *a* calculated at density functional theory level 317 (2000) 547
- Sundqvist, B., see Liu, B. 320 (2000) 365
- Sundström, V., see Tarnovsky, A.N. 312 (1999) 121
- Suo, Z., Y. Zhang, J.M. Zheng, Z. Xu, C. Li and Z. Bai, Generation and characterization of $C_{60}(CN)_2^{n-}$ ($n = 1, 2, 3$) 315 (1999) 321
- Surján, P.R., see Kállay, M. 312 (1999) 221
- Susnow, R.G., A.M. Dean and W.H. Green Jr., Hydrogen abstraction rates via density functional theory 312 (1999) 262
- Suter, H.U., J.R. Huber and T.-K. Ha, Photodissociation of carbonyl cyanide $CO(CN)_2$. An ab initio calculation study 311 (1999) 474
- Sutmann, G., see Balucani, U. 315 (1999) 109

- Suzuka, I., see Sanekata, M. 312 (1999) 422
- Suzuki, E., see Yamaguchi, Y. 316 (2000) 477
- Suzuki, T., see Akasaka, T. 319 (2000) 153
- Suzuki, Y., Y. Takasaki, Y. Tominaga and O. Mishima, Low-frequency Raman spectra of amorphous ices 319 (2000) 81
- Sykes, M.J., see McCoy, E.F. 313 (1999) 707
- Szafrański, M. and A. Katrusiak, Thermodynamic behaviour of bistable $\text{NH}^+ - \text{N}$ hydrogen bonds in monosalts of 1,4-diazabicyclo[2.2.2]octane 318 (2000) 427
- Szöke, A., Time-resolved holographic diffraction at atomic resolution 313 (1999) 777
- Szubiakowski, J., A. Balter, W. Nowak, K. Wisniewski and K. Aleksandrak, Substituent-sensitive anisotropic rotations of 9-acetoxy-10-phenylanthracenes: fluorescence anisotropy decay and quantum-mechanical study 313 (1999) 473
- Szwarc, H., see Senyavin, V.M. 313 (1999) 421
- Szwarc, H., see Céolin, R. 314 (1999) 21
- Szwarc, H., see Allouchi, H. 317 (2000) 40
- Tabata, K., see Yamaguchi, Y. 316 (2000) 477
- Tachibana, A., see Sakata, K. 320 (2000) 527
- Tachikawa, H., see Shimizu, A. 314 (1999) 516
- Tachimori, S., see Erkoç, Ş. 314 (1999) 203
- Tada, T., see Robinson, A.P.G. 312 (1999) 469
- Tagami, A., see Kohtani, S. 316 (2000) 88
- Tai, Y., see Yamaguchi, W. 311 (1999) 341
- Tajima, N., see El-Nahas, A.M. 318 (2000) 333
- Takabayashi, Y., see Inoue, T. 316 (2000) 381
- Takaichi, S., see Akimoto, S. 313 (1999) 63
- Takami, S., see Shrivastava, K.N. 313 (1999) 279
- Takano, Y., see Soda, T. 319 (2000) 223
- Takasaki, Y., see Suzuki, Y. 319 (2000) 81
- Takatsuka, K., see Yanao, T. 313 (1999) 633
- Takayanagi, T., Y. Kurosaki, K. Yokoyama, K. Sato and S. Tsunashima, Theoretical calculations of thermal rate constants for the $\text{N}(^2\text{D}) + \text{acetylene}$ reaction 312 (1999) 503
- Takeo, H., see Abe, H. 311 (1999) 153
- Takeo, H., see Ingólfsson, O. 311 (1999) 421
- Takeuchi, K., see Onoe, J. 315 (1999) 19
- Takezoe, H., see Manaka, T. 317 (2000) 260
- Takigawa, Y., see Akiyama, K. 317 (2000) 490
- Takizawa, M., see Yudasaka, M. 312 (1999) 155
- Talbi, D., An extensive ab initio study of a process of astrophysical interest: the $\text{N}^+(\text{N}) + \text{CH}_3(\text{CH}_3^+)$ reaction 312 (1999) 291
- Talbi, D., An extensive ab-initio study of the $\text{C} + \text{NH}_2$ and $\text{N} + \text{CH}_2$ reactions in relation to the HCN/HNC space abundance ratios 313 (1999) 626
- Talebpour, A., A.D. Bandrauk, J. Yang and S.L. Chin, Multiphoton ionization of inner-valence electrons and fragmentation of ethylene in an intense Ti:sapphire laser pulse 313 (1999) 789
- Tamarit, J.LI., see Allouchi, H. 317 (2000) 40
- Tan, T.L., K.L. Goh, P.P. Ong and H.H. Teo, High-resolution Fourier transform infrared spectroscopy and analysis of the ν_{12} fundamental band of ethylene- d_4 315 (1999) 82
- Tanabe, K., see Tsuzuki, S. 319 (2000) 547

- Tanaka, H., see Yokoyama, K. 320 (2000) 645
- Tanaka, K., see Ito, A. 315 (1999) 348
- Tanaka, M. and T. Kushida, Studies of the vibronic interaction between Eu^{3+} ions and glass-forming units in oxide glasses 315 (1999) 428
- Tanaka, N., see Naito, M. 319 (2000) 71
- Tanemura, S., see Yamaguchi, W. 311 (1999) 341
- Tanemura, S., see Yamaguchi, W. 311 (1999) 415
- Tang, J., Y. Sumiyoshi and Y. Endo, Detection of the triplet HC_4N radical by Fourier transform microwave spectroscopy 315 (1999) 69
- Tang, K., see Lu, Q. 314 (1999) 37
- Tang, K.T., see Sachse, T.I. 317 (2000) 346
- Tang, X.-J., see Wu, L.-Z. 315 (1999) 379
- Tang, Y.H., Y.F. Zhang, H.Y. Peng, N. Wang, C.S. Lee and S.T. Lee, Si nanowires synthesized by laser ablation of mixed SiC and SiO_2 powders 314 (1999) 16
- Taniguchi, Y., see Fueno, H. 312 (1999) 65
- Tanimoto, Y., see De, R. 315 (1999) 383
- Tanimura, Y., see Okumura, K. 314 (1999) 488
- Tao, F.-M., see Li, Z. 313 (1999) 313
- Tapia, O., see Safont, V.S. 318 (2000) 361
- Tardivel, B., see Piuze, F. 320 (2000) 282
- Tarnovsky, A.N., J.-L. Alvarez, A.P. Yartsev, V. Sundström and E. Åkesson, Photodissociation dynamics of diiodomethane in solution 312 (1999) 121
- Tashkun, S.A., see Tyuterev, V.I.G. 316 (2000) 271
- Tatchen, J. and C.M. Marian, On the performance of approximate spin-orbit Hamiltonians in light conjugated molecules: the fine-structure splitting of HC_6H^+ , NC_5H^+ , and NC_4N^+ 313 (1999) 351
- Taylor, H.S., see Belkić, D. 315 (1999) 135
- Teat, S.J., see Jones, R.H. 319 (2000) 423
- Tedesco, E., see Lanning, O.J. 317 (2000) 296
- Tekely, P., see Potrzebowski, M.J. 313 (1999) 569
- Tennyson, J., see Császár, A.G. 312 (1999) 613
- Tennyson, J., see Kain, J.S. 317 (2000) 365
- Teo, H.H., see Tan, T.L. 315 (1999) 82
- Ter-Avetisyan, S., see Ban, T. 313 (1999) 110
- Teraishi, K., see Shrivastava, K.N. 313 (1999) 279
- Terazima, M., see Ukai, A. 319 (2000) 427
- Teredesai, P.V., A.K. Sood, D.V.S. Muthu, R. Sen, A. Govindaraj and C.N.R. Rao, Pressure-induced reversible transformation in single-wall carbon nanotube bundles studied by Raman spectroscopy 319 (2000) 296
- Terenziani, F., see Painelli, A. 312 (1999) 211
- Terrones, H., see Hsu, W.K. 317 (2000) 77
- Terrones, M., see Hsu, W.K. 317 (2000) 77
- Teule, J.M., G.C. Groenenboom, D.W. Neyer, D.W. Chandler and M.H.M. Janssen, State-to-state photodynamics of nitrous oxide and the effect of long-range interaction on the alignment of $\text{O}(\text{D}_2)$ 320 (2000) 177
- Texier, I., J.-F. Delouis, J.A. Delaire, C. Giannotti, P. Plaza and M.M. Martin, Dynamics of the first excited state of the decatungstate anion studied by subpicosecond laser spectroscopy 311 (1999) 139

- Theil Kuhn, L., see Bouwen, W. 314 (1999) 227
- Thiel, W., see Breidung, J. 313 (1999) 713
- Thimm, G., see Winkler, B. 312 (1999) 536
- Thomas, D.S., see Kim, J.S. 315 (1999) 307
- Thompson, C.J., see Aguirre, F. 318 (2000) 466
- Thompson, D.E., see Rector, K.D. 316 (2000) 122
- Thomsen, C.L., see Mayer, S.G. 314 (1999) 246
- Thorne, J.R.G., C.S. McCaw and R.G. Denning, Spin-correlated crystal field analysis of lanthanide elpasolites 319 (2000) 185
- Thummel, R.P., see Nosenko, Y. 315 (1999) 87
- Thune, E., see Cabioc'h, T. 320 (2000) 202
- Thyssen, J., see Kellö, V. 318 (2000) 222
- Tian, S.R., see Furukawa, K. 318 (2000) 22
- Tian, S.X., see Chen, X.J. 319 (2000) 76
- Tian, Z.-Q., see Xu, X. 311 (1999) 193
- Tian, Z.Q., see Cao, P.G. 316 (2000) 1
- Titmuss, S.J., P.L. Cummins, A.A. Bliznyuk, A.P. Rendell and J.E. Gready, Comparison of linear-scaling semiempirical methods and combined quantum mechanical/molecular mechanical methods applied to enzyme reactions 320 (2000) 169
- Titze, A., see Böhmer, R. 316 (2000) 419
- Tobin, R.G., see Hsu, C.-L. 316 (2000) 336
- Toennies, J.P., see Sachse, T.I. 317 (2000) 346
- Tokhadze, K.G., see Mielke, Z. 316 (2000) 108
- Tokmakoff, A., see Okumura, K. 314 (1999) 488
- Tokumoto, H., see Lantz, M.A. 315 (1999) 61
- Tomas, A. and R. Lesclaux, Self-reaction kinetics of the $(\text{CH}_3)_2\text{CHC}(\text{O})\text{O}_2$ and $(\text{CH}_3)_3\text{CC}(\text{O})\text{O}_2$ acylperoxy radicals between 275 and 363 K 319 (2000) 521
- Tominaga, Y., see Suzuki, Y. 319 (2000) 81
- Tominaga, Y., see Amo, Y. 320 (2000) 703
- Tomita, S., M. Hikita, M. Fujii, S. Hayashi and K. Yamamoto, A new and simple method for thin graphitic coating of magnetic-metal nanoparticles 316 (2000) 361
- Tommei, G.E., see Ferrando, R. 315 (1999) 153
- Tonokura, K., S. Marui and M. Koshi, Absorption cross-section measurements of the vinyl radical in the 440-460 nm region by cavity ring-down spectroscopy 313 (1999) 771
- Tonokura, K., T. Murasaki and M. Koshi, Diagnostics of the gas-phase thermal decomposition of Si_2H_6 using vacuum ultraviolet photoionization 319 (2000) 507
- Topp, M.R., see Palmer, P.M. 318 (2000) 440
- Towrie, M., see Griffiths, P.T. 315 (1999) 158
- Tretiak, S., see Chernyak, V. 319 (2000) 261
- Troisi, A., see Fowler, P.W. 312 (1999) 77
- Trommsdorff, H.P., see Plazanet, M. 320 (2000) 651
- Truong, T.-T.T., see Truong, T.N. 314 (1999) 529
- Truong, T.N. and T.-T.T. Truong, A reaction class approach with the integrated molecular orbital + molecular orbital methodology 314 (1999) 529
- Truong, T.N., see Shapovalov, V. 320 (2000) 186
- Tsai, C.Y., see Wen, T.C. 311 (1999) 173
- Tsai, P.-C., see Wei, T.-H. 318 (2000) 53

- Tschirschwitz, F. and E.T.J. Nibbering, Femtosecond pump–probe and grating scattering study of condensed-phase hydrogen-bonding dynamics of complexes of Coumarin 102 312 (1999) 169
 Tschirschwitz, F., see Fiedor, L. 319 (2000) 145
 Tse, J.S., see Liu, Z.F. 311 (1999) 93
 Tse, J.S., see Liu, Z.F. 314 (1999) 317
 Tseng, H.C., see Nee, J.B. 318 (2000) 402
 Tsuchida, E., Y. Kanada and M. Tsukada, Density-functional study of liquid methanol 311 (1999) 236
 Tsukada, M., see Tsuchida, E. 311 (1999) 236
 Tsunashima, S., see Takayanagi, T. 312 (1999) 503
 Tsunoyama, H., K. Ohshimo, Y. Yamakita, F. Misaizu and K. Ohno, Photoionization and density functional theory study of clusters of acetone containing an alkali metal atom, $M((CH_3)_2CO)_n$ ($M = Li, Na$): intracuster electron transfer from metal to acetone in 1:1 complexes 316 (2000) 442
 Tsurusawa, T. and S. Iwata, Theoretical studies of the water-cluster anions containing the OH(e)HO structure: energies and harmonic frequencies 315 (2000) 433
 Tsuruya, H., see Shrivastava, K.N. 313 (1999) 279
 Tsuyumoto, I., see Ito, K. 318 (2000) 1
 Tsuzuki, S., T. Uchimaru, K. Matsumura, M. Mikami and K. Tanabe, Effects of the higher electron correlation correction on the calculated intermolecular interaction energies of benzene and naphthalene dimers: comparison between MP2 and CCSD(T) calculations 319 (2000) 547
 Tsuzuki, S., see Uchimaru, T. 318 (2000) 203
 Tuchagues, J.-P., see Bousseksou, A. 318 (2000) 409
 Tuckett, R.P., see Jarvis, G.K. 315 (1999) 287
 Tuckett, R.P., see Jarvis, G.K. 320 (2000) 104
 Tully, C., see Sokolovski, D. 313 (1999) 225
 Tung, C.-H., see Wu, L.-Z. 315 (1999) 379
 Turi, L., P. Mináry and P.J. Rossky, Non-linear response and hydrogen bond dynamics for electron solvation in methanol 316 (2000) 465
 Turner, G.W., see Lanning, O.J. 317 (2000) 296
 Turner, J.F.C., see Carter, V.J. 313 (1999) 505
 Turowska-Tyrk, I., see Graja, A. 313 (1999) 725
 Turski, P., On the ground states of copper, silver and gold silicides 315 (1999) 115
 Turukhin, A.V. and A.A. Gorokhovskiy, Determination of quantum efficiency of persistent spectral hole burning using dispersive kinetics 317 (2000) 109
 Tuzun, R.E., see Noid, D.W. 316 (2000) 285
 Tyuterev, V.I.G., S.A. Tashkun, D.W. Schwenke, P. Jensen, T. Cours, A. Barbe and M. Jacou, Variational EKE-calculations of rovibrational energies of the ozone molecule from an empirical potential function 316 (2000) 271
 Ubachs, W., see Scheper, C.R. 312 (1999) 131
 Uchimaru, T., J. Korchowiec, S. Tsuzuki, K. Matsumura and S. Kawahara, Importance of secondary electrostatic interactions in hydrogen-bonding complexes: an investigation using the self-consistent charge and configuration method for subsystems 318 (2000) 203
 Uchimaru, T., see Chandra, A.K. 318 (2000) 69
 Uchimaru, T., see Tsuzuki, S. 319 (2000) 547
 Uebayasi, M., see Kitaura, K. 312 (1999) 319
 Uebayasi, M., see Kitaura, K. 313 (1999) 701
 Uebayasi, M., see Nakano, T. 318 (2000) 614

- Uesu, Y., see Kato, N. 312 (1999) 115
- Ugliengo, P., B. Civalieri, C.M. Zicovich-Wilson and R. Dovesi, H-Chabazite with variable Si/Al ratio: stability and OH vibrational frequency computed in a periodic LCAO B3-LYP approach 318 (2000) 247
- Ukai, A., N. Hirota and M. Terazima, Radical diffusion measured by the transient grating in a short timescale 319 (2000) 427
- Uličný, J. and A. Laaksonen, Hypericin, an intriguing internally heterogenous molecule, forms a covalent intramolecular hydrogen bond 319 (2000) 396
- Ullrich, S., see Dessent, C.E.H. 319 (2000) 375
- Umanskii, I.M., see Eryomin, V.V. 316 (2000) 303
- Umbach, E., see Hopmeier, M. 314 (1999) 9
- Umemoto, H., $^{14}\text{N}/^{15}\text{N}$ isotope effect in the UV photodissociation of N_2O 314 (1999) 267
- Umemura, J., see Miura, Y. 315 (1999) 1
- Umemura, J., see Hasegawa, T. 317 (2000) 644
- Umeuchi, S., see Ohta, N. 315 (1999) 151
- Unnikrishnan, R., see Selvan, R. 316 (2000) 205
- Unno, O., see Amano, T. 311 (1999) 433
- Urahata, S. and S. Canuto, Monte Carlo study of the temperature dependence of the hydrophobic hydration of benzene 313 (1999) 235
- Urbasch, G., see Harrison, M.G. 313 (1999) 755
- Uruga, T., see Inoue, T. 316 (2000) 381
- Vaca Chávez, F., see Pusiol, D.J. 312 (1999) 91
- Vach, H., E. Fort, A. De Martino, M. Châtelet and F. Pradère, Structure-dependent evaporation dynamics for the surface scattering of binary Van der Waals clusters 314 (1999) 552
- Vala, J., see Wang, Z. 313 (1999) 155
- Valdés, H., V.M. Rayón and J.A. Sordo, The tetrahydropyran \cdots HCl dimer: a theoretical study 320 (2000) 507
- Valiente, R., O. Wenger and H.U. Güdel, New photon upconversion processes in Yb^{3+} doped CsMnCl_3 and RbMnCl_3 320 (2000) 639
- Vallauri, R., see Balucani, U. 315 (1999) 109
- Vallauri, R., see Jedlovsky, P. 318 (2000) 155
- Van Alsenoy, C., see Miao, M.S. 316 (2000) 297
- Van Caillie, C. and R.D. Amos, Geometric derivatives of density functional theory excitation energies using gradient-corrected functionals 317 (2000) 159
- Vander Auwera, J., see Herregodts, F. 316 (2000) 460
- Van der Auweraer, M., see Scheblykin, I.G. 316 (2000) 37
- Van der Auweraer, M., see Pevenage, D. 319 (2000) 512
- Van der Auweraer, M., see Jin, Y.D. 320 (2000) 387
- Van der Avoird, A., see Rode, M. 314 (1999) 326
- Van der Meer, M.J., H. Zhang, W. Rettig and M. Glasbeek, Femto- and picosecond fluorescence studies of solvation and non-radiative deactivation of ionic styryl dyes in liquid solution 320 (2000) 673
- Van Doren, V.E., see Miao, M.S. 316 (2000) 297
- Vanhoutte, F., see Bouwen, W. 314 (1999) 227
- Van Oijen, A.M., see Durand, Y. 317 (2000) 232
- Van Santen, R.A., see Ciobică, I.M. 311 (1999) 185

- Van Smaalen, S., R.E. Dinnebier, R. Milletich, M. Kunz, I. Holleman, G. von Helden and G. Meijer, Compressibility of CO intercalated C_{60} crystals 319 (2000) 283
- Van Tendeloo, G., see Willems, I. 317 (2000) 71
- Van Tendeloo, G., see Colomer, J.-F. 317 (2000) 83
- Van Voorhis, T. and M. Head-Gordon, The imperfect pairing approximation 317 (2000) 577
- Varandas, A.J.C. and Z.R. Xu, On the behavior of single-surface nuclear wavefunctions in the vicinity of the conical intersection for an X_3 system 316 (2000) 248
- Vardeny, Z.V., see Lee, C.W. 314 (1999) 564
- Varnavski, O. and T. Goodson III, Femtosecond fluorescence dynamics and molecular interactions in a water-soluble nonlinear optical polymeric dye 320 (2000) 688
- Varret, F., see Bousseksou, A. 318 (2000) 409
- Väterlein, P., see Föhlisch, A. 315 (1999) 194
- Vatsa, R.K., see Dhanya, S. 318 (2000) 125
- Vaval, N., Molecular properties using bi-orthogonal functional: a de-coupled scheme 318 (2000) 168
- Vázquez, S.A., see Martínez-Núñez, E. 316 (2000) 471
- Vecchiocattivi, F., see Ohoyama, H. 313 (1999) 484
- Vega, S., see Vinogradov, E. 314 (1999) 443
- Vega, S., see Goldbourt, A. 320 (2000) 448
- Velino, B., S. Melandri, P.G. Favero, A. Dell'Erba and W. Caminati, Rotational spectrum of 1,1-difluoroethane–argon: influence of the interaction with the Ar atom on the V_3 barrier to internal rotation of the methyl group 316 (2000) 75
- Veluri, K., see Arteca, G.A. 319 (2000) 719
- Venegas, V., J. Ortiz-López, G. Rueda-Morales and F. Caleyo, Synthesis and characterization of Hg metal-doped C_{60} 318 (2000) 655
- Vener, M.V. and J. Sauer, Quantum anharmonic frequencies of the $O \cdots H \cdots O$ fragment of the $H_3O_2^+$ ion: a model three-dimensional study 312 (1999) 591
- Ventura, E., A.M. Simas and D. Bazeia, Exact topological twistons in crystalline polyethylene 320 (2000) 587
- Verdal, N., J.T. Godbout, T.L. Perkins, G.P. Bartholomew, G.C. Bazan and A.M. Kelley, Raman and site-selective fluorescence spectra of model compounds for interchain interactions in poly(phenylenevinylene) 320 (2000) 95
- Verdasco, E., see Martínez-Haya, B. 311 (1999) 159
- Vergès, J., see Amiot, C. 315 (1999) 55
- Vergès, J., see Amiot, C. 318 (2000) 289
- Versluis, C., see Sarobe, M. 313 (1999) 31
- Vierheilig, A., T. Chen, P. Waltner, W. Kiefer, A. Materny and A.H. Zewail, Femtosecond dynamics of ground-state vibrational motion and energy flow: polymers of diacetylene 312 (1999) 349
- Vigliotti, F., see Jeannin, C. 316 (2000) 51
- Vijayakumar, V., see Rao, R. 313 (1999) 749
- Vijaya Sarathy, K., K.S. Narayan, J. Kim and J.O. White, Novel fluorescence and morphological structures in gold nanoparticle–polyoctylthiophene based thin films 318 (2000) 543
- Villareal, P., see Gianturco, F.A. 311 (1999) 255
- Villarreal, P., see Buchachenko, A.A. 318 (2000) 578
- Vincent, M.A., L.D. Salsi and I.H. Hillier, NO reduction: reaction of a readily formed intermediate $(NO)_3$ or $(NO)_3^-$ 314 (1999) 138
- Vincent, M.A., see Hall, R.J. 320 (2000) 139
- Vinogradov, E., P.K. Madhu and S. Vega, High-resolution proton solid-state NMR spectroscopy by phase-modulated Lee–Goldburg experiment 314 (1999) 443

- Vitukhnovsky, A.G., see Scheblykin, I.G. 316 (2000) 37
- Vivekananda, S., see Srinivas, R. 316 (2000) 243
- Vivien, L., E. Anglaret, D. Riehl, F. Bacou, C. Journet, C. Goze, M. Andrieux, M. Brunet, F. Lafonta, P. Bernier and F. Hache, Erratum to "Single-wall carbon nanotubes for optical limiting". [Chemical Physics Letters 307 (1999) 317-319] 312 (1999) 617
- Vogler, A., see Kunkely, H. 319 (2000) 486
- Voigt, B., see Fiedor, L. 319 (2000) 145
- Volkov, A.V., see Abramov, Yu.A. 311 (1999) 81
- Volkov, V., see Mohamed, M.B. 317 (2000) 519
- Von Helden, G., see Remmers, K. 317 (2000) 197
- Von Helden, G., see van Smaalen, S. 319 (2000) 283
- Vrinceanu, D., A.Z. Msezane and D. Bessis, A new expansion in \hbar : accurate calculations of Regge trajectories for singular potentials 311 (1999) 395
- Waclawik, E.R., see Legon, A.C. 312 (1999) 385
- Wadehra, J.M., see Reid, D.D. 311 (1999) 385
- Wägberg, T., see Liu, B. 320 (2000) 365
- Wahl, E.H., see Zhao, M. 318 (2000) 555
- Wahl, E.H., see Lommatzsch, U. 320 (2000) 339
- Wakahara, T., see Akasaka, T. 319 (2000) 153
- Walbert, S., see Fodor, L. 316 (2000) 411
- Wallington, T.J., O.J. Nielsen and K. Sehested, Kinetics of the reaction of CH_3O_2 radicals with NO_2 313 (1999) 456
- Walther, T., see McIntosh, A. 314 (1999) 57
- Waltner, P., see Vierheilig, A. 312 (1999) 349
- Walton, D.R.M., see Hsu, W.K. 317 (2000) 77
- Waluk, J., see Dobkowski, J. 318 (2000) 79
- Wang, D., see Zhu, X. 319 (2000) 85
- Wang, F., G. Hong and L. Li, A simplified scheme for relativistic density functional computation in the zeroth-order regular approximation 316 (2000) 318
- Wang, F., see Ke, X.Z. 313 (1999) 40
- Wang, F., see Deng, J.K. 313 (1999) 134
- Wang, G.-J., see Zhu, R. 313 (1999) 98
- Wang, H.-L., D.W. McBranch, V.I. Klimov, R. Helgeson and F. Wudl, Controlled unidirectional energy transfer in luminescent self-assembled conjugated polymer superlattices 315 (1999) 173
- Wang, L.-J., see Xu, W.-G. 314 (1999) 300
- Wang, L.-S., see Gutsev, G.L. 312 (1999) 598
- Wang, L.-S., see Wang, X.-B. 313 (1999) 179
- Wang, N., see Tang, Y.H. 314 (1999) 16
- Wang, N., see Zhang, Y. 317 (2000) 504
- Wang, N., see Zhou, X.T. 318 (2000) 58
- Wang, P., K. Komaguchi and M. Shiotani, An ESR and ab-initio MO study of $\pi_{\text{CH}_2-n_0}$ orbital crossover in cycloalkylketone radical cations 320 (2000) 623
- Wang, P., see Zhu, P. 311 (1999) 306
- Wang, S., W. Huang, H. Yang, Q. Gong, Z. Shi, X. Zhou, D. Qiang and Z. Gu, Large and ultrafast third-order optical non-linearity of single-wall carbon nanotubes at 820 nm 320 (2000) 411
- Wang, S.L., see Xu, S.C. 313 (1999) 617

- Wang, S.Y., see Nee, J.B. 318 (2000) 402
- Wang, W., see Guo, L. 318 (2000) 49
- Wang, X. and Q.-Z. Qin, A theoretical study of SN_2O_2 isomers 320 (2000) 144
- Wang, X., see Kelly, K.F. 313 (1999) 445
- Wang, X., see Sun, Z. 318 (2000) 471
- Wang, X.-B. and L.-S. Wang, Vibrationally resolved photoelectron spectroscopy of PO_3^- and the electronic structure of PO_3 313 (1999) 179
- Wang, X.-B., see Gutsev, G.L. 312 (1999) 598
- Wang, X.D., see Deng, J.K. 313 (1999) 134
- Wang, Y., Z. Gan, K. Su and Z. Wen, An improved externally contracted CI method 312 (1999) 277
- Wang, Y., see Deng, J.K. 313 (1999) 134
- Wang, Y.L., see Mebel, A.M. 318 (2000) 27
- Wang, Z., T. Wasserman, E. Gershgoren, J. Vala, R. Kosloff and S. Ruhman, Geminate recombination of I_3^- in cooled liquid and glassy ethanol 313 (1999) 155
- Wang, Z.L., see Li, D.-C. 316 (2000) 349
- Wang, Z.X., see Ke, X.Z. 313 (1999) 40
- Waplak, S., see Graja, A. 313 (1999) 725
- Wardlaw, D., see Jin, B. 317 (2000) 464
- Wark, A., see Kolmakov, A. 319 (2000) 465
- Washizu, H. and K. Kikuchi, Anisotropy of the electrical polarizability of a model DNA fragment in aqueous salt solution 320 (2000) 277
- Wasserman, T., see Wang, Z. 313 (1999) 155
- Watanabe, Y., see Onaka, K. 315 (1999) 75
- Wategaonkar, S., see Patwari, G.N. 316 (2000) 433
- Weaver, M.J., see Zou, S. 312 (1999) 101
- Wegmann, G., B. Schweitzer, D. Hertel, H. Giessen, M. Oestreich, U. Scherf, K. Müllen and R.F. Mahrt, The dynamics of gain-narrowing in a ladder-type π -conjugated polymer 312 (1999) 376
- Wei, T.-H., T.-H. Huang and T.-C. Wen, Mechanism of reverse saturable absorption in chloro-aluminum phthalocyanine solution studied with Z-scan 314 (1999) 403
- Wei, T.-H., T.-H. Huang, T.-T. Wu, P.-C. Tsai and M.-S. Lin, Studies of nonlinear absorption and refraction in C_{60} /toluene solution 318 (2000) 53
- Wei, T.-X., Y.-R. Shi, J. Zhai, L.-B. Gan, C.-H. Huang, T.-T. Liu, L.-M. Ying, G.-B. Luo and X.-S. Zhao, Synthesis, monolayer fabrication and photoelectric conversion property of two pyrrolidinofullerene carboxylic acid derivatives 319 (2000) 7
- Wei, X.M., see Zou, Z. 312 (1999) 149
- Weidele, H., see Bouwen, W. 314 (1999) 227
- Weinert, M., see Heinze, S. 315 (1999) 167
- Weingärtner, H., see Oleinikova, A. 319 (2000) 119
- Weiss, W., see Joseph, Y. 314 (1999) 195
- Wen, T.-C., see Wei, T.-H. 314 (1999) 403
- Wen, T.C. and C.Y. Tsai, Influence of azasubstitution on the nonlinear absorption in porphyrazine derivatives 311 (1999) 173
- Wen, Z., see Wang, Y. 312 (1999) 277
- Wenger, O., see Valiente, R. 320 (2000) 639
- Wenju, C., see Dong, X. 318 (2000) 433
- Werncke, W., see Hogiu, S. 312 (1999) 407
- Werner, H.-J., see Manthe, U. 313 (1999) 647
- Werner, H.-J., see Schütz, M. 318 (2000) 370

- Werner, R., see Ostrovsky, S.M. 320 (2000) 295
- Wesolowski, T.A., Application of the DFT-based embedding scheme using an explicit functional of the kinetic energy to determine the spin density of Mg^+ embedded in Ne and Ar matrices 311 (1999) 87
- Westley, M.S., see Pisano, P.J. 318 (2000) 385
- Wheatley, R.J., see Domene, C. 314 (1999) 158
- White, J.O., see Vijaya Sarathy, K. 318 (2000) 543
- Whiteley, T.W.J. and A.J. McCaffery, Classical and near-classical origins of the oscillations in state- and angle-resolved inelastic scattering 314 (1999) 132
- Wild, U.P., see Sepiol, J. 311 (1999) 29
- Wild, U.P., see Harms, G.S. 313 (1999) 533
- Wilde, R.E., see Bryans, T.R. 314 (1999) 459
- Willems, I., Z. Kónya, J.-F. Colomer, G. Van Tendeloo, N. Nagaraju, A. Fonseca and J. B.Nagy, Control of the outer diameter of thin carbon nanotubes synthesized by catalytic decomposition of hydrocarbons 317 (2000) 71
- Willems, I., see Colomer, J.-F. 317 (2000) 83
- Williams, K.A. and P.C. Eklund, Monte Carlo simulations of H_2 physisorption in finite-diameter carbon nanotube ropes 320 (2000) 352
- Williams, V.C., see Sloan, J. 316 (2000) 191
- Wilson, C.C., see Jones, R.H. 319 (2000) 423
- Wilson, M., see Domene, C. 314 (1999) 158
- Wilson, P.J., R.D. Amos and N.C. Handy, Toward coupled-cluster accuracy in the prediction of nuclear shielding constants: a simple and efficient DFT approach 312 (1999) 475
- Wimperis, S., see McManus, J. 311 (1999) 292
- Winkler, B., C.J. Pickard, V. Milman, W.E. Klee and G. Thimm, Prediction of a nanoporous sp^2 -carbon framework structure by combining graph theory with quantum mechanics 312 (1999) 536
- Winkler, T., see Ottinger, Ch. 314 (1999) 411
- Wisniewski, E.S., see Folmer, D.E. 318 (2000) 637
- Wisniewski, K., see Szubiakowski, J. 313 (1999) 473
- Woeller, M., see Filatov, M. 316 (2000) 135
- Wolf, M., see Bartels, L. 313 (1999) 544
- Wolff, M., see Kolmakov, A. 319 (2000) 465
- Wolfrum, J., see Schäfer, J. 319 (2000) 477
- Wolter, K., D. Scarano, J. Fritsch, H. Kuhlenbeck, A. Zecchina and H.-J. Freund, Observation of a localized surface phonon on an oxide surface 320 (2000) 206
- Wong, K.S., see Lee, C.W. 314 (1999) 564
- Wong, N.B., see Zhang, R.Q. 319 (2000) 213
- Wong, N.B., see Cheng, L.F. 319 (2000) 418
- Wong, T.C., see Zhang, X.H. 320 (2000) 77
- Woo, E.P., see Hofmann, U. 311 (1999) 41
- Wormer, P.E.S., see Rode, M. 314 (1999) 326
- Wright, J.S., see DiLabio, G.A. 311 (1999) 215
- Wright, P.A., see Carter, V.J. 313 (1999) 505
- Wright, T.G., see Soldán, P. 313 (1999) 379
- Wright, T.G., see Lee, E.P.F. 318 (2000) 196
- Wu, C.-X., see Iwamoto, M. 312 (1999) 7
- Wu, C.-X., see Zhao, W. 312 (1999) 572

- Wu, D.Y., see Xu, X. 311 (1999) 193
 Wu, F., see Nosenko, Y. 315 (1999) 87
 Wu, G. and K. Yamada, Residual dipolar couplings in MAS and MQMAS NMR spectra of quadrupolar nuclei 313 (1999) 519
 Wu, G., see Ji, Z. 311 (1999) 467
 Wu, G., see Ji, Z. 319 (2000) 45
 Wu, J. and Y. Jiang, Optimization of basis sets in valence bond calculations 311 (1999) 315
 Wu, L.-Z., X.-J. Tang, M.-H. Jiang and C.-H. Tung, Two-photon induced fluorescence of novel dyes 315 (1999) 379
 Wu, S.K., see Zhang, X.H. 320 (2000) 77
 Wu, T.-T., see Wei, T.-H. 318 (2000) 53
 Wu, W.W., see Hofmann, U. 311 (1999) 41
 Wu, Z., see Guo, L. 318 (2000) 49
 Wudl, F., see Wang, H.-L. 315 (1999) 173
 Wurth, W., see Föhlich, A. 315 (1999) 194
 Wurth, W., see Lau, J.T. 317 (2000) 269
 Wyatt, R.E., Quantum wavepacket dynamics with trajectories: wavefunction synthesis along quantum paths 313 (1999) 189
 Wyatt, R.E., see Minehardt, T.J. 312 (1999) 485

 Xenides, D. and G. Maroulis, Basis set and electron correlation effects on the first and second static hyperpolarizability of SO_2 319 (2000) 618
 Xia, B.-Y., see Cai, W.-S. 319 (2000) 708
 Xia, Z., see Qian, W. 319 (2000) 89
 Xian, H., see Xu, X. 311 (1999) 193
 Xiang, J., C. Chen, B. Zhou and G. Xu, Abnormal fluorescence behavior of some cyanine dyes in a cyanine dye- TiO_2 colloids system 315 (1999) 371
 Xie, D., see Parsons, B. 320 (2000) 499
 Xie, J.C., see Chen, X.L. 318 (2000) 107
 Xie, Q., G. Archontis and S.S. Skourtis, Protein electron transfer: a numerical study of tunneling through fluctuating bridges 312 (1999) 237
 Xie, R.H. and Q. Rao, Third-order optical nonlinearities of chiral graphene tubules 313 (1999) 211
 Xie, Y., H.F. Schaefer III and G.H. Robinson, The gallium-gallium triple bond in a realistic model. A density functional theory study of $\text{Na}_2[(\text{C}_6\text{H}_5)_2\text{C}_6\text{H}_3\text{GaGaC}_6\text{H}_3(\text{C}_6\text{H}_5)_2]$ 317 (2000) 174
 Xing, D., see Zhang, N. 313 (1999) 69
 Xu, C., see Sloan, J. 316 (2000) 191
 Xu, C.K., see Chen, X.J. 319 (2000) 76
 Xu, G., see Xiang, J. 315 (1999) 371
 Xu, G., see Jin, Z. 318 (2000) 505
 Xu, G.Q., see Zou, Z. 312 (1999) 149
 Xu, K.Z., see Chen, X.J. 319 (2000) 76
 Xu, S.C., R. Guo and S.L. Wang, Research on the model reactions of ClONO_2 with HCl on water clusters 313 (1999) 617
 Xu, W.-G., G.-L. Li, L.-J. Wang, S. Li and Q.-S. Li, Ab initio and density functional theory study of the mechanism of synthesis of the N_5^+ cation 314 (1999) 300
 Xu, X., D.Y. Wu, B. Ren, H. Xian and Z.-Q. Tian, On-top adsorption of hydrogen at platinum electrodes: a quantum-chemical study 311 (1999) 193

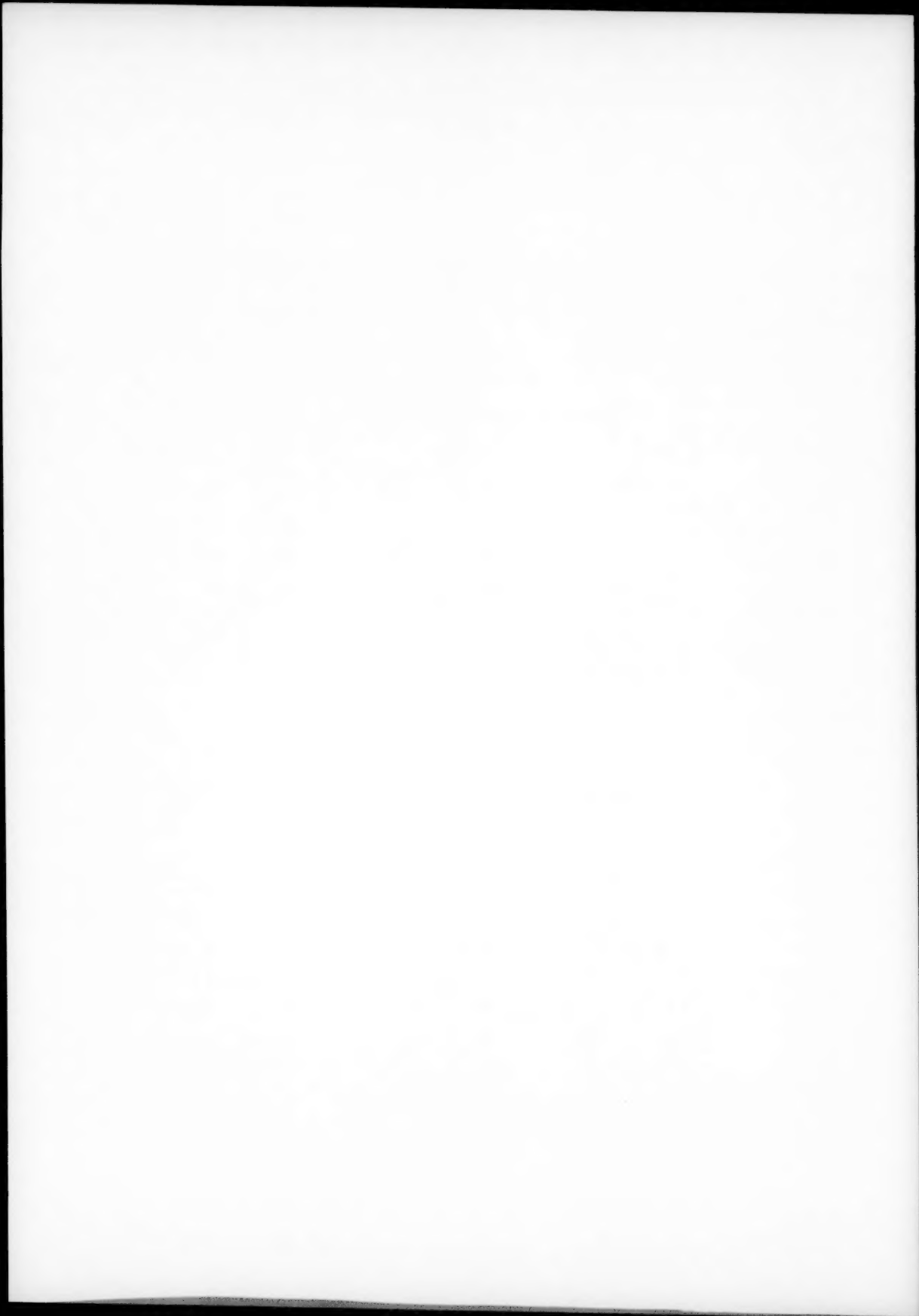
- Xu, Z., see Suo, Z. 315 (1999) 321
- Xu, Z.-F., see Yu, X. 320 (2000) 123
- Xu, Z.R., see Varandas, A.J.C. 316 (2000) 248
- Yabushita, S., see Yasuike, T. 316 (2000) 257
- Yagi, M., see Ochimizu, T. 313 (1999) 451
- Yamada, K., see Wu, G. 313 (1999) 519
- Yamada, K.M.T., see Abe, H. 311 (1999) 153
- Yamada, S., see Nakano, M. 311 (1999) 221
- Yamaguchi, K., see Nakano, M. 311 (1999) 221
- Yamaguchi, K., see Shigeta, Y. 315 (1999) 441
- Yamaguchi, K., see Nakano, M. 317 (2000) 103
- Yamaguchi, K., see Soda, T. 319 (2000) 223
- Yamaguchi, T., see Mahara, H. 317 (2000) 23
- Yamaguchi, W., K. Yoshimura, Y. Tai, Y. Maruyama, K. Igarashi, S. Tanemura and J. Murakami, Energy-controlled depositions of size-selected silver nanoparticles on HOPG substrates 311 (1999) 341
- Yamaguchi, W., K. Yoshimura, Y. Maruyama, K. Igarashi, S. Tanemura and J. Murakami, Non-destructive deposition and diffusion-aggregation of size-selected silver nanoclusters on glassy carbon substrates as probed by real-time X-ray photoelectron spectroscopy 311 (1999) 415
- Yamaguchi, Y., Y. Nagasawa, S. Shimomura, K. Tabata and E. Suzuki, A density functional theory study of the interaction of oxygen with a reduced SnO₂ (110) surface 316 (2000) 477
- Yamakita, Y., see Tsunoyama, H. 316 (2000) 442
- Yamamoto, K., see Tomita, S. 316 (2000) 361
- Yamamoto, K., see Akasaka, T. 319 (2000) 153
- Yamamoto, S., G.H.F. Diercksen and M. Karelson, An ab initio CI study of electronic spectra of substituted free-base porphyrins 318 (2000) 590
- Yamane, Y., see Ye, J.Y. 320 (2000) 607
- Yamashita, K., see Harima, Y. 317 (2000) 310
- Yamato, M., see Ohoyama, H. 313 (1999) 484
- Yamauchi, H., see Furukawa, K. 318 (2000) 22
- Yamauchi, M., see Ye, J.Y. 320 (2000) 607
- Yamazaki, I., see Akimoto, S. 313 (1999) 63
- Yamazaki, I., see Ohta, N. 315 (1999) 151
- Yamazaki, S., see Furukawa, K. 318 (2000) 22
- Yan, Y., see Zhang, Y. 317 (2000) 504
- Yan, Z.-C., see Zhu, J.-M. 313 (1999) 184
- Yanagimoto, M., see Mukai, K. 311 (1999) 446
- Yanao, T. and K. Takatsuka, Timescale of isomerization reactions and isotropic inflation model of basin boundaries in cluster dynamics 313 (1999) 633
- Yáñez, M., see Luna, A. 320 (2000) 129
- Yang, C., see Noid, D.W. 316 (2000) 285
- Yang, D.-S. and J. Miyawaki, Zero kinetic energy spectroscopy of AlNH₃ complex 313 (1999) 514
- Yang, H., see Liu, B. 320 (2000) 365
- Yang, H., see Wang, S. 320 (2000) 411
- Yang, J., see Talebpour, A. 313 (1999) 789
- Yang, J.-P., W. Paa and S. Rentsch, Femtosecond investigations of photophysics of ultrafast intersystem crossing in terthiophene by wavelength dependent excitation 320 (2000) 665

- Yang, J.P., see Jin, Y.D. 320 (2000) 387
- Yang, Q., see Dai, Z. 317 (2000) 9
- Yang, R., see Liu, B. 320 (2000) 365
- Yang, W., see Zhang, N. 313 (1999) 69
- Yang, Z.-Z., see Cong, Y. 316 (2000) 324
- Yao, J.L., see Cao, P.G. 316 (2000) 1
- Yao, N., see Hsu, W.K. 317 (2000) 77
- Yaremko, A.M., see Ratajczak, H. 314 (1999) 122
- Yartsev, A.P., see Tarnovsky, A.N. 312 (1999) 121
- Yartsev, V.M., Electronic correlation and electron-molecular vibration coupling effects on non-linear optical properties of molecular dimer 313 (1999) 241
- Yasuike, T. and S. Yabushita, Valence photoionization and autoionizing states of acetylene studied by the complex basis function method in the random phase approximation 316 (2000) 257
- Ye, C., see Zhu, P. 311 (1999) 306
- Ye, J.Y., Y. Yamane, M. Yamauchi, H. Nakatsuka and M. Ishikawa, Direct observation of the interaction of single fluorescent nucleotide analogue molecules with DNA polymerase I 320 (2000) 607
- Ye, P., see Dai, Z. 317 (2000) 9
- Ye, T., E. Gershgoren, N. Friedman, M. Ottolenghi, M. Sheves and S. Ruhman, Resolving the primary dynamics of bacteriorhodopsin, and of a ' $C_{13}=C_{14}$ locked' analog, in the reactive excited state 314 (1999) 429
- Yeh, F.-F., see Hsu, C.-C. 311 (1999) 355
- Yencha, A.J., G.C. King, M.C.A. Lopes, J.D. Bozek and N. Berrah, Photo-double ionization of deuterium chloride studied by threshold photoelectrons coincidence spectroscopy 315 (1999) 37
- Yersin, H., see Homeier, H.H.H. 316 (2000) 280
- Yethiraj, A., see Egorov, S.A. 317 (2000) 560
- Yin, M. and J.-C. Krupa, Superfluorescence from $NdCl_3$ 314 (1999) 27
- Ying, L.-M., see Wei, T.-X. 319 (2000) 7
- Yokoyama, K., N. Haketa, M. Hashimoto, K. Furukawa, H. Tanaka and H. Kudo, Production of hyperlithiated Li_2F by a laser ablation of $LiF-Li_3N$ mixture 320 (2000) 645
- Yokoyama, K., see Takayanagi, T. 312 (1999) 503
- Yoon, J.H., see Nam, K.-Y. 319 (2000) 391
- York, A.P.E., see Sloan, J. 316 (2000) 191
- Yoshii, N., R. Miyauchi, S. Miura and S. Okazaki, A molecular-dynamics study of the equation of state of water using a fluctuating-charge model 317 (2000) 414
- Yoshii, T., see Ito, A. 315 (1999) 348
- Yoshikawa, K., see Mayama, H. 318 (2000) 113
- Yoshimoto, T., see Ohta, Y. 316 (2000) 551
- Yoshimura, K., see Yamaguchi, W. 311 (1999) 341
- Yoshimura, K., see Yamaguchi, W. 311 (1999) 415
- Yoshioka, Y., see Soda, T. 319 (2000) 223
- Yu, H.-G. and G. Nyman, An application of the rotating line umbrella model to quantum dynamics of S_N2 reactions 312 (1999) 585
- Yu, J., see Chang, R. 317 (2000) 142
- Yu, J., see Chang, R. 317 (2000) 153
- Yu, N.-T., see Li, W.-H. 312 (1999) 28
- Yu, X., S.-M. Li, J.-Y. Liu, Z.-F. Xu, Z.-S. Li and C.-C. Sun, Direct ab initio dynamics studies of the hydrogen abstraction reaction: $AsH_3 + H \rightarrow AsH_2 + H_2$ 320 (2000) 123

- Yu, Y., St.J. Dixon-Warren and N. Astle, Molecular-beam study of the adsorption and desorption of hydrogen sulfide on Ag{111} 312 (1999) 455
- Yudasaka, M., N. Sensui, M. Takizawa, S. Bandow, T. Ichihashi and S. Iijima, Formation of single-wall carbon nanotubes catalyzed by Ni separating from Y in laser ablation or in arc discharge using a C target containing a NiY catalyst 312 (1999) 155
- Yudasaka, M., see Suenaga, K. 316 (2000) 365
- Yue, X., see Dai, Z. 317 (2000) 9
- Zachariasse, K.A., Comment on "Pseudo-Jahn-Teller and TICT-models: a photophysical comparison of *meta*- and *para*-DMABN derivatives" [Chem. Phys. Lett. 305 (1999) 8]. The PICT model for dual fluorescence of aminobenzonitriles 320 (2000) 8
- Zanasi, R., Resolution of molecular electric hyperpolarizabilities into atomic terms 315 (1999) 217
- Zang, Q.J., see Lu, W.C. 311 (1999) 491
- Zanuy, D., see Alemán, C. 319 (2000) 318
- Zapater, I., see Martínez-Haya, B. 311 (1999) 159
- Zare, R.N., see Zhao, M. 318 (2000) 555
- Zare, R.N., see Lommatzsch, U. 320 (2000) 339
- Zarić, S.D., Cation- π interaction with transition-metal complex as cation 311 (1999) 77
- Zazubovich, N., see Babin, V. 314 (1999) 31
- Zazubovich, S., see Babin, V. 314 (1999) 31
- Zecchina, A., see Wolter, K. 320 (2000) 206
- Zei, M.S., see Lin, W.F. 312 (1999) 1
- Zenevich, V.A., G.D. Billing and G. Jolicard, Vibrational-rotational energy transfer in H_2-H_2 collisions. II. The relative roles of the initial rotational excitation of both diatoms 312 (1999) 530
- Zenobi, R., see Stöckle, R.M. 318 (2000) 131
- Zerbetto, F., see Buma, W.J. 313 (1999) 426
- Zerbi, G., see Mapelli, C. 314 (1999) 189
- Zerulla, D., D. Mayer, K.H. Hallmeier and T. Chassé, Angular-resolved XANES measurements of the polar and azimuthal orientation of alkanethiols on InP(110) 311 (1999) 8
- Zettl, A., see Cumings, J. 316 (2000) 211
- Zettl, A., see Cumings, J. 318 (2000) 497
- Zettl, A., see Ishigami, M. 319 (2000) 457
- Zewail, A.H., see Vierheilig, A. 312 (1999) 349
- Zgierski, M.Z., see Siebrand, W. 320 (2000) 153
- Zhabotinsky, A.M., see Kurin-Csörgei, K. 311 (1999) 105
- Zhai, J., see Wei, T.-X. 319 (2000) 7
- Zhang, C.H., see Chen, X.L. 318 (2000) 107
- Zhang, D., F. Liang, D. Feng and C. Liu, Ab initio study of the reorganization barrier for bent triatomic species 317 (2000) 430
- Zhang, F.S., see Ke, X.Z. 313 (1999) 40
- Zhang, H., see Zhu, R. 313 (1999) 98
- Zhang, H., see Van der Meer, M.J. 320 (2000) 673
- Zhang, J.P., see Hsu, W.K. 317 (2000) 77
- Zhang, L., see Zhou, M. 318 (2000) 644
- Zhang, N., W. Yang, G. Li, W. Ding, D. Xing and Y. Du, Sintering temperature-dependent magnetism and structure in granular perovskites $La_{1-x}Sr_xMnO_3$ 313 (1999) 69

- Zhang, Q., see Zhang, Y. 317 (2000) 504
- Zhang, R., see Lee, S.-H. 315 (1999) 7
- Zhang, R.Q., N.B. Wong, S.T. Lee, R.S. Zhu and K.L. Han, Computation of large systems with an economic basis set: a density functional study on proton-bound carboxylic acid clusters 319 (2000) 213
- Zhang, R.Q., see Zhu, R.S. 320 (2000) 561
- Zhang, S., see Liu, B. 320 (2000) 365
- Zhang, X., see Lu, J. 312 (1999) 85
- Zhang, X., see Zhang, Y. 317 (2000) 504
- Zhang, X.H., W.Y. Lai, Z.Q. Gao, T.C. Wong, C.S. Lee, H.L. Kwong, S.T. Lee and S.K. Wu, Photoluminescence and electroluminescence of pyrazoline monomers and dimers 320 (2000) 77
- Zhang, Y., J. Zhu, Q. Zhang, Y. Yan, N. Wang and X. Zhang, Synthesis of GeO_2 nanorods by carbon nanotubes template 317 (2000) 504
- Zhang, Y., see Suo, Z. 315 (1999) 321
- Zhang, Y.A., see Deng, J.K. 313 (1999) 134
- Zhang, Y.F., see Tang, Y.H. 314 (1999) 16
- Zhao, M., E.H. Wahl, T.G. Owano, C.C. Largent, R.N. Zare and C.H. Kruger, Near-surface reduction of cavity ring-down spectroscopy detection sensitivity 318 (2000) 555
- Zhao, Q., see Piuze, F. 320 (2000) 282
- Zhao, W., C.-X. Wu and M. Iwamoto, Rate-equation theory of azobenzene monolayer photoisomerization 312 (1999) 572
- Zhao, X., see Lu, J. 312 (1999) 85
- Zhao, X.-S., see Wei, T.-X. 319 (2000) 7
- Zhao, X.S., see Jiang, H. 319 (2000) 555
- Zheng, J.M., see Suo, Z. 315 (1999) 321
- Zheng, X. and D.L. Phillips, Substituent and solvent effects on the short-time A-band photodissociation dynamics of CF_2I_2 313 (1999) 467
- Zheng, X. and D.L. Phillips, Density functional theory and resonance Raman investigation of the ultraviolet electronic excited states of CF_2I_2 316 (2000) 524
- Zheng, X.-Y., A. Harata and T. Ogawa, Fluorescence photon bursts from low surface-density dioctadecyl-rhodamine B molecules at the air-water surface observed with a confocal fluorescence photon-counting microscope 316 (2000) 6
- Zheng, Y., see Deng, J.K. 313 (1999) 134
- Zhong-can, O.-Y., see Iwamoto, M. 312 (1999) 7
- Zhong, J., see Chen, Z. 313 (1999) 217
- Zhou, B., see Xiang, J. 315 (1999) 371
- Zhou, B.-L., see Zhu, J.-M. 313 (1999) 184
- Zhou, G., see Lu, Q. 314 (1999) 37
- Zhou, L., Ab initio and density functional predictions of the structure, gas-phase acidity and aromaticity of 1,2-dithio-3,4-diselenosquaric acid 317 (2000) 330
- Zhou, M., Z. Fu, L. Zhang and Q. Qin, Structure and stability of LiOMn molecule generated by laser ablation 318 (2000) 644
- Zhou, W., see Collins, C. 312 (1999) 346
- Zhou, X., see Wang, S. 320 (2000) 411
- Zhou, X.T., H.L. Lai, H.Y. Peng, F.C.K. Au, L.S. Liao, N. Wang, I. Bello, C.S. Lee and S.T. Lee, Thin $\beta\text{-SiC}$ nanorods and their field emission properties 318 (2000) 58
- Zhou, Y., S. Constantine, J.A. Gardecki and L.D. Ziegler, Dispersed ultrafast nonresonant electronic responses: detuning oscillations and near resonance effects 314 (1999) 73

- Zhu, C. and C. Lifshitz, The protonated betaine/ammonia complex: how stable is the gas-phase zwitterion structure? 320 (2000) 513
- Zhu, H., see Guo, L. 318 (2000) 49
- Zhu, H.-S., see Fu, Q. 314 (1999) 223
- Zhu, J., see Zhang, Y. 317 (2000) 504
- Zhu, J.-M., B.-L. Zhou and Z.-C. Yan, Dispersion coefficients for interactions among two-electron atomic systems 313 (1999) 184
- Zhu, L. and T.J. Cronin, Photodissociation of benzaldehyde in the 280-308 nm region 317 (2000) 227
- Zhu, P., P. Wang and C. Ye, Theoretical investigation on the first hyperpolarizability of push-pull polyenes containing non-aromatic cyclic olefines 311 (1999) 306
- Zhu, R., H. Zhang, G.-J. Wang, X. Gu, K.-L. Han, G.-Z. He and N.-Q. Lou, Photodissociation of *o*-bromotoluene at 266 nm 313 (1999) 98
- Zhu, R.S., R.Q. Zhang and K.S. Chan, Carbon nitride formation in gas-phase reactions of CH₄, NH₃ and H₂: an ab initio study 320 (2000) 561
- Zhu, R.S., see Zhang, R.Q. 319 (2000) 213
- Zhu, X., M. Ge, C. Qiao, Z. Sun and D. Wang, A HeI photoelectron spectrum of the (CH₃CH₂CH₂)₂N radical 319 (2000) 85
- Zhu, X.D., see Nabighian, E. 316 (2000) 177
- Zhu, Y.Q., see Hsu, W.K. 317 (2000) 77
- Zhu, Z.Y., see Ke, X.Z. 313 (1999) 40
- Zicovich-Wilson, C.M., see Ugliengo, P. 318 (2000) 247
- Ziegler, L.D., see Zhou, Y. 314 (1999) 73
- Zietz, B., see Rettig, W. 317 (2000) 187
- Zilberberg, I., see Pelmenchikov, A. 314 (1999) 496
- Zilio, S.C., see Dos Santos Jr., D.S. 317 (2000) 1
- Zilker, S.J., see Hofmann, U. 311 (1999) 41
- Zimmermann, H., see Ernst, M. 317 (2000) 583
- Zobov., N.F., see Császár, A.G. 312 (1999) 613
- Zojer, E., see Knupfer, M. 318 (2000) 585
- Zou, G., see Liu, B. 320 (2000) 365
- Zou, S. and M.J. Weaver, Surface-enhanced Raman spectroscopy of cadmium sulfide/cadmium selenide superlattices formed on gold by electrochemical atomic-layer epitaxy 312 (1999) 101
- Zou, Y., see Qian, W. 319 (2000) 89
- Zou, Z., X.M. Wei, Q.P. Liu, H.H. Huang, W.S. Sim, G.Q. Xu and C.H.A. Huan, Interaction of atomic hydrogen, HS and H₂S on GaAs(100) 312 (1999) 149
- Zubarev, R.A., see Budnik, B.A. 316 (2000) 19
- Zubek, M., see Mielewska, B. 311 (1999) 428
- Zúñiga, J., A. Bastida, M. Alacid and A. Requena, Global potential energy surfaces for the CO₂ and CS₂ molecules 313 (1999) 670
- Zuppiroli, L., see Donzé, N. 315 (1999) 405



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